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Improving life cycle assessment methodology for the application of decision support
Focusing on the statistical value chain

Herrmann, Ivan Tengbjerg; Hauschild, Michael Zwicky

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- Focusing on the statistical value chain

Ivan T. Herrmann

PhD Thesis, April, 2012

DTU Management Engineering
Institut for Systemer, Produktion og Ledelse

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Author: Ivan T. Herrmann

DTU Management Engineering
Produktionstorvet, building 426
DK-280 Kgs. Lyngby

Phone: +45 2275 6975
Email: ivan.t.h.business@gmail.com

Print: Schultz Grafik A/S

"People care about the decisions you make, but they care even more about the process you used along the way."

- from Change Management (Kim & Mauborgne 2003)

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1 Preface

This PhD project has been performed in the period from January 2009 to April 2012, including a 6 month research stay at Lawrence National Laboratory Berkeley with Professor Tom McKone. The PhD project is part of a larger project (the Project platform) conducted by: Novozymes A/S; Biochemical Engineering (DTU); Department of Management Engineering, Technical University of Denmark (DTU); Department of Molecular Biology (UAA); Emmelev A/S; and the Danish National Advanced Technology Foundation. The focus for the Project platform has been to develop an enzymatic transesterification process for producing biodiesel, which should be more sustainable and economically superior to the conventional transesterification process. This PhD project has contributed to the sustainability assessment of biodiesel from a life cycle perspective, including different types of transesterification processes. This PhD dissertation presents a summary and a common thread of my main findings during the project period. The main findings for this PhD project are presented in articles that I have produced and submitted during this project. These articles are presented in their entirety in appendices A to D. In addition, findings that were not included in these articles are presented in this PhD dissertation. In the appendix additional material that I find relevant for this PhD thesis are also presented, such as conference and seminar presentations.

1.1 Acknowledgments

I would like to thank my supervisor Professor Michael Hauschild, Postdoc Andreas Jørgensen, Section secretary Christine Molin, Associate Professor Jørgen Lindgaard Pedersen (all from Department of Management Engineering, DTU); Professor Tom McKone and Senior researcher Michael Sohn (Lawrence National Laboratory Berkeley); Professor Henrik Spliid (Department of Informatics and Mathematical Modeling, DTU); Novozymes; and The Danish National Advanced Technology Foundation for their useful comments, motivational support, and making this PhD project economically possible.

Kgs. Lyngby, April 12, 2012

Ivan T. Herrmann

2 Summary

There have been two overall objectives for this PhD thesis:

a) To improve the life cycle assessment (LCA) methodology for the application of decision support and evaluation of uncertainty in LCA.
b) LCA of biodiesel from a well-to-wheel (WTW) perspective.

<u>Improving the LCA methodology for the application of decision support and evaluation of uncertainty in LCA.</u>

From a decision maker's (DM's) point of view there are at least three main "illness" factors influencing the quality of the information that the DM uses for making decisions. The factors are not independent of each other, but it seems helpful to use the following separations for clarification:

- Uncertainty
- Costs
- Time

Improvements in just one of these three factors can swiftly lead to an improvement of the others since they are highly dependent on each other. The focus of this PhD project has been on uncertainty.

Most application-oriented LCAs are used as an "overall linking" decision support tool, meaning that they summarize relatively large amounts of data mainly collected in the literature (e.g. articles, various databases and reports), which rarely gives anything other than point estimates (such as an average value). Previous methods for evaluation of uncertainties in LCA have mainly been based on estimates from experts and variation expansion, for example by using Monte Carlo simulation.

The methods and theories upon which this PhD thesis is based are mainly from the management literature (especially the *rational* school of management) and the statistical literature.

My suggestion for improved LCA methodology is based on what I regard as the "*statistical value chain*", which is summarized below. Understanding the statistical value chain will increase the

possibility for DMs, LCA experts, analysts (ANs), etc., to pinpoint where uncertainties may arise in LCA.

The statistical value chain

The world is as it is at any given time (P_t). How the world was at $P_{t\text{-}1\ \ldots\ t\text{-}m}$ is undeniable. Prospectively we presume to influence how the world will be for $P_{t+1\ldots t+n}$.

Step 1: *Defining the population that will be investigated*: For information about the world, we need to collect empirical data. We cannot collect data on the entire world, but we need to collect data on the population(s) that we are making enquiries into. The starting point of a data collecting process is to *outline* (or define) the population that will be investigated, both with regard to space and time.

Step 2: *Full investigation/Theory of Sampling (TOS)*: When a population has been defined, we then have two options for seeking information: A) seek full information (i.e., examine each population as a whole) or B) use representative sampling and then generalize to the full population that the LCA used for decision support aims to describe. Only well-used sampling procedures described by TOS can lead to representative sampling of population(s). TOS is often used to as a method to save resources compared to investigating the complete population.

Step 3: *Descriptive statistics*: Descriptive statistics is about computing averages, variation analysis, minimums and maximums, distributions, etc. of the different populations investigated in step 2.

Step 4: *The retrospective LCA*: As long as a given LCA can be categorized as a retrospective assessment it is, in this PhD thesis, assumed that LCA is a matter of accounting and based on the previous steps this accounting is, more or less, straight forward and the accounting should cover the total LCA system, i.e. all populations. This step is analogous to a company's financial statement.

Step 5: *Developing the baseline for prospective LCA*: The first step in prospective assessment is to construct a baseline, which can be characterized by: "*exactly what (you think) will happen if the change under consideration was not introduced*" (business-as-usual). The following step (step 6) outlines methods for the prospective LCA.

Step 6: *Inferential statistics*: By the use of inferential statistics we can construct models, i.e. establish relationships and correlations between the different populations investigated in the previous steps. Based on the model developed we can produce forecasts/predictive analysis for $P_{t+1 \ldots t+n}$.

Step 7: *Alternatives*: All relevant alternatives to the baseline study in step 5. The difference between the baseline study and alternatives provide the potentials for improvements/changes (both positive and negative).

Step 8: *Valuation*: Here, valuation is meant as a sum of all humans' utility of the conditions given/estimated in steps 1-7.

The statistical value chain should not be interpreted as a rigid procedure where the AN starts at "step 1" and ends at "step 8". The process of developing an LCA used for decision support is an iterative process with an ex-ante (*priori*) to the LCA project start unknown number of N-steps, going back and forth between the different steps.

A deterioration of the quality in each step is likely to accumulate through the statistical value chain in terms of increased uncertainty and bias. Ultimately this can make final decision support problematic.

The "Law of large numbers" (LLN) is the methodological tool/probability theory that has been used consistently throughout this PhD thesis and forms the basis for evaluating the inherent uncertainty in different types of LCAs. The LLN is here interpreted as: "*the larger a sample (n) from a given population is, the more accurate the estimate of the true average of the population (N) will be*". Furthermore, I have assumed that *N* can be interpreted as the LCA *space* that we are making LCA statements about. An LCA statement is the answer to an LCA question (or inquiry). Based on the LLN it can be seen that reducing uncertainties in LCA is probably not possible to do in ways other than to A) use more resources on a given analysis, or B) reduce the size of the LCA space into which inquiries are made.

The above statistical value chain together with LLN is explored in the article "Confronting uncertainty in LCA used for decision support", which is submitted to the *Journal of Industrial Ecology*. This article presents a simple but powerful, methodical tool (a pedigree matrix) to assess and potentially confront uncertainties in LCA based on a developed taxonomy used for classification of different types of LCAs. Use of this tool may lead to an increased transparency (or reduced obscurity) for the DM through a potentially quick identification of "*what is included in the LCA and what is not*". It is also discussed in this article that the *accepted* uncertainty level is decision support context depending and also personal. This may then cause the situation where some DMs completely (or partially) refrain from making a decision based on an LCA and thus support a decision on other parameters than the LCA environmental parameters. Conversely, it may in some decision support contexts be acceptable to base a decision on highly uncertain information. This all depends on the specific decision support context and it is not possible to derive objective rules about what one *ought* to do. This is the "*is-ought*" problem as formulated by the Scottish philosopher David Hume in 1739. For example, it is an "*is*-issue" what the uncertainty in a given information is (from a statistically point-of-view), but it is an "*ought*-issue" whether the DM ought to base a decision on information with a high/low degree of inherent uncertainty. In the article "Does it matter which LCA tool you choose? - comparative assessment of SimaPro and GaBi on a biodiesel case study", which has been submitted to the *International Journal of Life Cycle Assessment*, it is shown that already by step 4 in the statistical value chain there can be considerable uncertainties in an applied LCA used for decision support.

LCA of biodiesel from a WTW perspective

This PhD project has two main stakeholders: Emmelev A/S (biodiesel producer) and Novozymes A/S (enzyme producer), both with the goal of developing an enzymatic transesterification process that would be environmentally preferable compared to the current conventional alkaline transesterification process. Based on the data available during the project period, it has not been possible to demonstrate that an enzymatic transesterification process (evaluated on a CO_2–eq. emission scale) is preferable compared to the conventional process. However, given that the enzymatic process enables the use of bioethanol (instead of petrochemical methanol), then the enzymatic process improves biodiesel from a WTW perspective, i.e. the change from petrochemical methanol to bioethanol is a benefit that exceeds the negative effect of transitioning from a conventional to an enzymatic transesterification process. It should be kept in mind that the processes are compared as they are today without any attempt to predict further developments of either the enzymatic or the conventional process. The conventional process is a mature and well-developed process, in contrast to the enzymatic process, which is new and immature. We expect that the improvement potential for the enzymatic process is somewhat higher than for the conventional process. This is discussed in the article "Potentials for optimized production of biodiesel in a well-to-wheel study". This article also evaluates other environmental impact categories such as "Land Use" (based on the Recipe and IMPACT2002+ methodologies), "Respiratory inorganic," "Human toxicity (Carcinogenic)", "Ecotoxicity freshwater" (based on the USEtox^{TM} methodology), and “Aquatic acidification (N)” (based on the EDIP2003 methodology). This article has been submitted to the *International Journal of Life Cycle Assessment*.

In the above study the "Transesterification process" and "Use of alcohol for producing biodiesel" are used as explanatory variables for response variables such as "Global warming potential" or "Land use". In the event that one (or more) DM(s) are able to influence multiple explanatory variables, it may be interesting to analyze the various explanatory variables that have the potential for improvement on the different response variables and quantify the improvement potential. To enable such an analysis a method has been developed which I have named the "Structural LCA approach" based on "Design of Experiments" (DOE). The “Structural LCA approach” can lead to a large number of unique alternatives of different production methods (and uses). Each alternative we regard as being a pathway (PW): all PWs together form the LCA solution space while any additional PW will increase the LCA solution space. Given that this space is (relatively) large and that several response variables are to be evaluated simultaneously, then this can be characterized as a "multi-objective optimization" problem. A method for handling such a problem has been developed in collaboration with the “Operations Research” group at the Management Engineering department of the Technical University of Denmark. The suggested “Structural LCA approach” and derivative optimization issues are addressed in the article "Enabling optimization in LCA - from the to the Structural LCA approach". This article has been submitted to the *International Journal of Life Cycle Assessment*. This study also shows that for the production of biodiesel from a WTW perspective the explanatory variable that has the highest improvement potential for the global warming response variable is the "use of straw from the field," which can potentially be a substitute for coal for power generation in a power plant.

3 Dansk resumé

Der har været to overordnede mål for denne Ph.d.-afhandling:

a) At forbedre livscyklusvurdering (LCA) metodegrundlag. Det forbedrede LCA metodegrundlag har været fokuseret på LCA som beslutningsstøtteværktøj herunder involveret usikkerheder.
b) LCA af biodiesel i et ”produktion og brug” perspektiv (WTW-perpektiv).

Forbedret LCA metodegrundlag med fokus på beslutningsstøtte og usikkerhed i LCA

Fra en beslutningstagers synspunkt er der mindste tre ”illness” faktorer, der påvirker kvaliteten af de informationer som beslutningstageren basere en beslutning på. Faktorerne er ikke uafhængige af hinanden - men i det følgende, synes det hensigtsmæssigt at bruge følgende adskillelse:

- Usikkerhed
- Omkostninger
- Tid

Forbedringer af blot en af de tre faktorer, kan nemt føre til en forbedring af de andre faktorer, da de er meget afhængige af hinanden. Fokus i dette Ph.d.-projekt har været på usikkerhed.

Som udgangspunkt er de fleste anvendelsesorienterede LCA'er et ”overbygningsværktøj”, som sammenfatter en relativ stor mængde af data, der hovedsaligt er indsamlet i litteraturen, dvs. artikler, forskellige databaser og rapporter som sjældent giver andet end *punkt*-estimater, for eksempel et gennemsnit. Tidligere metoder til evaluering af usikkerheder i LCA har hovedsagligt været baseret på estimater fra eksperter og variationsekspansion, for eksempel ved brug af Monte Carlo simulering af sådanne ekspertestimater.

Mit forslag til forbedret LCA metodegrundlag kommer igennem, hvad jeg betragter som den ”*statistisk værdikæde*”, som er opsummeret nedenfor. Via en forståelse af den statistiske værdikæde, vil det øge indsigten og muligheden for at beslutningstagere m.fl. kan vurdere usikkerheder i LCA.

Den statistiske værdikæde

Det er antaget at verden til et givet tidspunkt (P_t), er som den er. Hvordan verden var ved $P_{t\text{-}1\ldots t\text{-}m}$ er uomtvisteligt og kun fremad rettet kan vi influere på verdens tilstand.

Trin 1: *Bestemmelse af population, der ønskes undersøgt*: For information om verden er vi nødt til at indsamle empiriske data. Naturligvis kan vi ikke indsamler data om hele verden, derfor er vi nødt til at indsamle data om en eller flere populationer som vi ønsker at udtale os om. Enhver data indsamlings procedure må starte med at skitsere (eller definere) den/de population(er), som ønskes undersøgt - både med hensyn til "rum og tid".

Trin 2: *Theory of Sampling* (TOS): Den/de populationer, som vi vil udtale os om, kan man enten A) søge fuld information om (dvs. undersøge hele populationen) *eller* B) informationer baseret på et *repræsentativt udsnit* af populationen og derpå generalisere til hele populationen. Kun vel anvendt sampling procedure, beskrevet ved TOS, kan lede til sådanne repræsentative samples af populationer. Den sidst nævnte metode (TOS) er den del af statistikken, som i princippet er udviklet til at spare ressourcer, så man ikke behøver at undersøge hele populationen (først nævnte procedure).

Trin 3: *Deskriptiv statistik*: I dette step beskrives de populationer, som der er indhentet data for for eksempel angives i dette step gennemsnitsværdier, variations (koefficienter) i populationer, min og max, fordelinger mv.

Trin 4: *Retrospektiv LCA*: Så længe en given LCA kan kategoriseres som en retrospektiv vurdering, antager jeg, at LCA er et spørgsmål om regnskab og baseret på de foregående trin er dette regnskab, mere eller mindre ligefremt, og regnskabet skal dække det samlede LCA produktionssystemet, dvs. alle inkluderet populationer. Dette step svarer til at lave et virksomhedsregnskab.

Trin 5: *Baseline studie for prospektive LCA'er*: Første skridt i en prospektiv LCA må være at konstruere en baseline, som bør være kendetegnet ved: "*hvad (du tror) vil ske, hvis de kommende ændring der er overvejet, ikke blev indført*" (business-as-usual). Følgende trin (trin 6) skitsere metoder til prospektiv LCAer baseret på inferential statistik.

Trin 6: *Inferential statistik*: Her bygges modeller, det vil sige opstilling af sammenhænge og korrelationer mellem de forskellige populationer. På baggrund af de opstillede modeller kan der laves forecasts/prediktive analyser for $P_{t+1 \ldots t+n}$.

Trin 7: *Alternativer*: Alle relevante alternativer til baseline studiet i trin 5. Differencen mellem baseline studiet og alternativer giver ændringspotentialet.

Trin 8: *Værdisætning*: her er værdisætning tænkt som en sum af alle menneskers værdi af de givende forhold som er givet/(estimeret i) trin 1-7.

Den statistiske værdikæde skal ikke forstås som en rigid procedure, hvor analytikeren starter på "trin 1" og slutter på "trin 8". Processen med at udvikle en LCA brugt til beslutningsstøtte vil jeg hævde er en iterativ proces med et *ex-ante* til LCA-projekt start ukendt antal af N-trin, hvor analytikeren bevæger sig frem og tilbage mellem de forskellige trin.

Det er klart, at hvis kvaliteten af de enkelte trin bliver kompromitteret i en given analyse, så vil dette ligeledes kompromittere kvaliteten af den endelige beslutningsstøtte. Endvidere vil en forringelse af kvaliteten i de enkelte trin, kunne ophobe sig op igennem den statistiske værdikæde, i form af øget usikkerhed, som i sidste ende kan være så betydningsfulde at reel beslutningsstøtte bliver problematisk.

Desuden er *"Law of large numbers"* (LLN) et gennemgående sandsynlighedsregnings/metodiskværktøj i denne Ph.d.-fremstilling, som bruges til at evaluere usikkerheder med. LLN bliver fortolket, i denne sammenhæng, således: *"med en fast sample størrelse (n) vil usikkerheden for en given analyse være voksende med et voksende størrelse på den undersøgte population (N)*". Det er endvidere antaget at (*N*) kan fortolkes som det "*LCA space*", som en analytiker udtaler sig om når resultatet af en LCA præsenteres for en beslutningstager. Dette fortolkes i denne Ph.d. som at jo større et LCA spac'et er som analytikeren udtaler sig om, jo mere usikkert vil resultatet af analysen være, givet at analytikeren har et endeligt antal ressourcer til rådighed. Det kan af LLN også ses at man næppe kan komme usikkerheder i LCA til livs på anden vis, end at bruge flere ressourcer på en given analyse (givet at "effektivitetsniveauet" for analytikeren er konstant) – eller mindske størrelsen på den mængde/population, man ønsker undersøgt.

Den ovenstående statistiske værdikæde sammen med LLN er reflekteret i artiklen Confronting Uncertainty in LCA", som er sendt til *Journal of Industrial Ecology*. Denne artikel angiver et simpelt, men stærkt, metodisk værktøj (en pedigree matrix) til at vurdere iboende usikkerheder i LCA med. Brugen af dette værktøj kan medføre øget gennemsigtighed for en beslutningstager i form af en hurtigere identifikation (end normalt) af: "*hvad der er medtaget i LCA og hvad der ikke er*". Det er i denne artikel ydereligere diskuteret, hvad beslutningsstøtte*konteksten* kan influere på selve beslutningsstøtten. For eksempel, må det også konstateres at den *accepterede* usikkerhed, det vil sige det niveau af usikkerhed, der kan accepteres af en person/beslutningstager når der skal træffes et valg mellem to alternativer, er beslutningsstøtte kontekst afhængig og herunder også personlig. Dermed kan der altså opstå den situation at en beslutningstager helt, eller delvist, afstår fra at træffe en beslutning på baggrund af et LCA studie, hvis beslutningstager finder LCA resultaterne for usikre. Dermed vil beslutningstagerens beslutninger blive baseret på helt andre parametre end LCA miljøparametre. Omvendt kan der også være beslutningsstøttekontekster hvor beslutningstager finder det nødvendigt at bruge information af miljøpåvirkninger selvom disse informationer er præget af høj usikkerhed. Det er dog ikke muligt at udlede et generelt regelsæt om hvad man *bør* gøre i en specifik beslutningsstøttekontekst. Den skotske filosof David Hume formulerede omkring 1739 "*the is-ought problem*", hvor han pointere at det ikke er muligt at gå fra "is" til "ought" uden at anvende subjektive regler. For eksempel, er det et "is-issue" hvad usikkerheden i en given information er (statistisk set), men det er et "ought-issue" om beslutningstager bør basere en beslutning på meget (eller lidt) usikre informationer. I artiklen "Does it matter which LCA tool you choose? - comparative assessment of SimaPro and GaBi on a biodiesel case study", der er sendt til *International Journal of Life Cycle Assessment*, er det vist at på et "trin 4" i den statistiske værdikæde, kan der forekomme betydelige usikkerheder i en anvendt LCA. Dette kan så betragtes som et "*is*-issue".

<u>LCA af biodiesel i WTW-perspektiv</u>

Ph.d.-projektet har haft to hovedinteressenter, Emmelev A/S (biodiesel producent) og Novozymes A/S (Enzym producent) begge med det mål at forbedre den eksisterende produktion af biodiesel. Målet har været at udvikle en enzymatisk transesterifikationsproces, som ville være miljømæssigt fortrukken sammenlignet med den nuværende konventionelle alkaliske transesterification proces. Med de data, der har været tilgængelige i projekt perioden, har det ikke været muligt at påvise at en enzymatisk transesterification proces (isoleret set), i et CO_2 emissions perspektiv, er at fortrække i forhold til den konventionelle proces. Givet at den enzymatiske proces muliggør brugen bioethanol (i stedet for petrokemisk metanol) vil dette dog forbedre biodiesel i et WTW perspektiv, det vil sige ændringen fra metanol til bioethanol er en fordel, som overgår den (meget lille ændring) som det vil være at gå fra den konventionelle proces til den enzymatiske proces. For denne konklusion skal der tages det forbehold at processerne er sammenlignet som de er *i dag*, uden forsøg på at forudsige udviklingsmulighederne for hverken den enzymatiske eller konventionelle proces. Den konventionelle proces er en *moden* og en veludviklet proces i modsætning til den enzymatiske proces, der er en ny og *umoden* proces. Umiddelbart forventer vi os fremadrettet et større forbedringspotentiale for den enzymatiske proces end for den konventionelle proces. Dette er behandlet i artiklen ”Potentials for optimized production of biodiesel in a well-to-wheel study”, som er baseret på state-of-the-art LCA, der også evaluerer miljøpåvirkningskategorierne ”Land Use” (baseret på ReCiPe og IMPACT2002+ metodologierne), “Respiratory inorganics”, “Human toxicity (carc)” og”Ecotoxicity freshwater” (baseret på USEtox^{TM} metodologien), Aquatic acidification (N) (baseret på EDIP2003 metodologien). Dette studie er sendt til the *International Journal of Life Cycle Assessment*.

I ovenstående studie betragtes ”transesterification proces” og ”brug af alkohol til at lave biodiesel”, som to forklarende variable (explanatory variables) for respons variablen/erne, for eksempel ”Global warming potential” eller ”Land use”. I det tilfælde at en (eller flere) beslutningstager(e) har mulighed for at ændre på mere end en forklarende variabel, kan det være interessant at kunne kvantificere og analysere, de forskellige forklarende variables indflydelse på de givende respons variable. For at nå hertil, er der udviklet en metode, som jeg har kaldt ”the Structural LCA approach”, der er baseret på ”Design of Experiments” (DOE). The Structural LCA approach lede til et stort antal unikke alternativer af forskellige produktionsmetoder (og brug). Hvert alternativ kalds for en pathway (PW), som giver en ekstra løsning i LCA løsnings*rummet*. Givet at dette løsningsrum bliver relativt stort og at flere respons variable skal evalueres samtidig, giver dette et problem af ”multiobjektive optimerings” karakter. Metoden the Structural LCA approach og afledte problemstillinger er behandlet i artiklen ”Enabling optimization in LCA from *ad hoc* to Structural LCA” Denne artikel er sendt til the *International Journal of Life Cycle Assessment*. I dette studie ses desuden at den forklarende variable, som mest markant kan ændre Global warming potentialet for biodiesel i et WTW perspektiv er ”brugen af strå fra marken”, som ved afbrænding i et kraftværk kan substituere kul.

4 Introduction

Life Cycle Assessment (LCA) offers a quantitative approach to evaluate different types of impacts of products, technologies and services (Wenzel, Hauschild & Alting 1997; Finnveden et al. 2009; EC-JRC 2010). LCAs are conducted by LCA practitioners or analysts (AN) to support decision makers (DMs) in making the best possible choice for the environment in a given situation. In general, the goal of LCA is to compare different approaches for providing the same functional unit (FU).

Sustainability is defined in the UN program by three dimensions: the environmental, the social, and the economical (un.org 2012). This PhD project focuses on the environmental dimension and the other two dimensions are not considered further in this dissertation.

4.1 The life cycle assessment methodology

LCA is a methodology which attempts to include all material inputs and outputs to and from the evaluated FU: the material extraction phase, product production phase, use phase, and disposal phase as well as transportation in all phases. The first step in a LCA is to collect all the data in the life cycle and compile an inventory of all the materials going in and out of the life cycle. Based on this inventory and characterization factors (CF) describing the environmental impact for all the different materials, an aggregated impact assessment of the product can be established (Wenzel, Hauschild & Alting 1997).

The goal of this PhD project has been two-fold:

a) Improve the LCA methodology for the application of decision support and evaluation of uncertainty in LCA.
b) Conduct an LCA of biodiesel from a well-to-wheel (WTW) perspective.

4.2 Improving the LCA methodology focusing on decision support and uncertainty.

From a DM’s point of view there are at least, three main “illness” factors influencing the quality of the information that the DM uses for decision making (Berger 1985; Lindley 1985; Royal Society

1992; Simonet & Wilde 1997; Montgomery 2005b). The factors are not independent of each other, but it is helpful to make the following distinctions for clarification:

- Uncertainty
- Costs
- Time

The illness factors are here understood as: the more uncertain the information, the higher the cost of the information, and the more time it takes to gather and present the information to the DM, the lower the quality of the decision support will be. In this PhD thesis, uncertainty is interpreted as the *probability* of a given event to occur, where probability is interchangeable with uncertainty. See Pitman (1993) for a formal treatment of probability theory. The probability for a given event to occur multiplied with the quantification of the actual event (e.g. emission of CO_2, the impact of a meteorite on Earth, or losing in the Lottery) is commonly treated in the literature as a *risk* (Oxford University Press 2011). DMs can have different risk attitudes (Royal Society 1992; Farmer et al. 1997; Simonet & Wilde 1997). Such DMs can be characterized as being either risk averse, risk neutral, or risk lovers (Estrin, David & Dietrich 2008). In this PhD thesis the focus is on the uncertainty part of this way of understanding risks. When using LCA as a decision support tool it is important to consider the implications and some of the different aspects of uncertainty when a DM chooses between different alternatives. Regarding costs, it seems obvious that a DM, which has a fixed budget, will also have cost preferences, hence this factor is also relevant for DMs (Keat 2009) and the application of LCA as a decision support tool. There are two aspects of "time" 1) the length of time it will take to make an LCA[1], and 2) when the result is delivered compared to an agreed point in time, as a specific date. The better the LCA practitioner can perform on both 1 and 2, the better decision support and hence improved decision making, can be expected.

Improvements in just one of the three factors outlined above can swiftly lead to an improvement in the other factors since they are highly dependent on each other. The focus in this PhD project is as mentioned on uncertainty.

From my early research in the literature on LCA of biodiesel it became clear that different LCA studies often arrived at quite different results for what seemed to be more or less the same product.

[1] Keeping the quality of the LCA result constant.

This issue has recently been addressed in Malça & Freire (2011). In general the LCA "picture" to some extent could seem to be muddy, at least when looking at different biodiesel studies.

In this PhD thesis it is assumed that LCA used for decision support, to a great extent, can be characterized as "information management", where the essential part are that 1) the AN gathers and summarizes information (such as specifying averages, expected values, min/max values variation(s) and so on) and 2) presents this information to the DM, who then makes a final decision. The less standardized the information is (or the more muddy the picture is) when it is presented to the DM, the more time consuming this process will be. This is due to the need for further explanation of general assumptions, LCA-specific assumptions, data collection strategies, etc. which are not familiar to the DM, before the DM can accept the conclusion and use the information in the context of a decision.

A) To me it then would seem to be value-adding to the general LCA field if a standardized and commonly accepted classification of different types of applied LCAs, used for decision support, could be developed to confront some of the problems described above and potentially reduce time and resources needed when the AN delivers LCA results and conclusions to the DM. Application of such a framework can be seen as a rapid way to increased transparency of the LCA work.

Another methodological challenge for LCA that became clear to me was the sometimes large uncertainty involved in LCA, which can influence the quality of the decision support. It is my impression that most of the LCA literature concerning uncertainties in LCA uses the following approach: "*given we have a result, how can we then calculate the uncertainty/certainty of this result?*" either based on an analytical approach or a simulation tool such as Monte Carlo.

B) Here it seemed reasonable, for me, to try to go the other way around and turn the process "upside down": "*if we want to quantify something, what would then be the most correct procedure for arriving at such result, to reduce the uncertainty as much as possible*". Deviation from this "correct procedure" would simply lead to an increased uncertainty and bias in the LCA results, which is not always possible to quantify in a meaningful way. The definition of the "correct procedure" can seem to be problematic, however much work has been done in the field of statistics to define procedures that are, at least, more correct than other procedures. I have assumed that knowledge from the statistical field can be an acceptable inspiration and benchmark for the LCA field.

A third methodological issue that became clear to me was that many LCA studies seemed to be using, what I would characterize as, an “*Ad Hoc” approach*.

C) If a more “structural” approach can be developed, one which clearly states what drives change within different impact categories and what their potential for environmental improvement are, then this would also be value-adding to the general LCA field.

The actual application of any of these three points (A, B, or C) can lead to a higher level of transparency compared to the present approach to applied LCAs. A higher level of transparency can potentially influence the uncertainty, cost, and time for applied LCAs used for decision support in a positive way. Point A, B, and C are broadly reflected in the four different papers that I have submitted during this PhD project.

4.3 LCA of biodiesel from a WTW perspective

This PhD project is part of a larger project (the Project platform) which is conducted by: Novozymes A/S; Biochemical Engineering (DTU); Department of Management Engineering, Technical University of Denmark (DTU); Department of Molecular Biology (UAA); Emmelev A/S; and the Danish National Advanced Technology Foundation. The focus for the Project Platform has been to develop an enzymatic transesterification process for producing biodiesel, which should be more sustainable and economically superior to the conventional transesterification process. The PhD project has contributed with sustainability assessment of biodiesel in a life cycle perspective.

The European Union has enacted a proposal that requires that each member state shall ensure that the share of energy from renewable sources in transport in 2020 is at least 10% of final consumption of energy (The European Parliament and the Council 2009). It is expected that in Europe the total energy consumption for transport in 2020 will be 438.6 Mtoe (ec.europa.eu 2008). The production of biodiesel in Europe in 2008 was 5.5 million tons (or 4.73 Mtoe) (Emerging-markets.com 2011).

As such the demand for energy from renewable sources is fixed and the main question that remains to be answered must be: *how to reach this target with the lowest possible environmental impact?*

As a framework to handle this problem, I have used use the Design of Experiments (DOE) methodology outlined in Montgomery (2005a) combined with LCA techniques. Different explanatory variables, such as transesterification processes, type of alcohol, and agriculture management, have been identified for the production and use of biodiesel, which potentially can give a better or worse response for the environmental impact categories.

The initial project was focused on the transesterification process where either an enzymatic or conventional transesterification can be applied. The other explanatory variables were used for benchmarking purposes of the environmental improvement potentials of the transesterification process.

Harding et al. (2008) developed an LCA of biodiesel production and compared enzymatic and conventional transesterification processes from a well-to-tank perspective with multiple impact categories and found that enzymatic biodiesel transesterification is environmentally advantageous compared to conventional biodiesel transesterification. Malça & Freire (2011) present a comprehensive review of 28 different LCA studies on biodiesel in Europe where all results are evaluated based on greenhouse gas (GHG) emissions per MJ. The two main issues raised in this study are the variability of results and the different modeling approaches between the different LCAs. The different modeling approaches are explained by different assumptions regarding geographical scope, the functional unit, multi-functionality (i.e. allocation problems), and agricultural modeling (mainly N_2O-emissions). Other modeling differences are also mentioned which we regard as "prospective", i.e. answering the questions of what *can* happen, opposite to studies of "the current situation" which is based on observable processes. The GHG emissions are reported to be ranging from 15 to 170 kg CO_2-eq./GJ. According to Howarth et al. (2009) very few biofuel studies report on environmental impacts other than GHGs.

Our study addresses multiple environmental impacts including: toxicity modeling based on the USEtox^{TM} methodology; nutrient balance calculations in the agricultural stage; land use; and the impact of indirect land use change (ILUC). Production data is based on empirical data from a Danish biodiesel producer. The modeling is based on state-of-the-art of current production technology, which can be considered as a benchmarking point for improvement on the already established biodiesel production and use in Europe. Furthermore, options for processes used in different biodiesel production steps that may reduce environmental impacts are investigated.

4.4 The structure of the PhD thesis

The sections in this PhD thesis, from (and including) the "**Title page**" and until the "**Methodologies and theory**" **section**, are considered as general formalities that require no further justification. Explanations for the different sections and structure of the rest of the PhD thesis (*main* text) from and including the Methods and theory section follows here.

The first chapter in the main text is "**Methodologies and theory**"**.** This chapter presents a brief introduction to the different methods and theories, and to some extent assumptions, that are used and underlying the output of this PhD thesis. In some cases it seems difficult to clearly distinguish between what a method is, what a theory is, and what an assumption is. Take for example sampling techniques, is it a method for collecting data in a correct way, is it a theory for how to collect data correctly – or is it just an assumption of what is the correct way to gather data? In some cases there might not be a meaningful distinction between these categories and no attempt has been made to elaborate further on this matter.

The second chapter in the main text is the "**Statistical value chain**". The statistical value chain is a description of the best (theoretical) procedure for collecting data, and building an LCA for decision support seen from a statistical perspective. I consider the Statistical value chain the core of this PhD thesis, forming a common thread throughout the PhD project. The next four chapters are based on the four papers that have been submitted in this PhD project and each paper is closely linked to the statistical value chain.

The third chapter in the main text is based on the submitted paper: "**Confronting Uncertainty in LCA used for decision support**". This paper outlines different types of LCAs often seen in the LCA literature but never explicitly identified. The different types of LCAs are ranked on an uncertainty scale in a pedigree matrix. The statistical value chain can be interpreted as the correct procedure to develop LCAs and when moving toward the lower left corner in the pedigree matrix (see Figure 1, page 41) the higher step in the statistical value chain is applied.

The fourth chapter in the main text is based on the submitted paper: "**Potentials for optimized production of biodiesel in a well-to-wheel study**". This paper is an LCA study of biodiesel production based on the lowest possible inherent uncertainty in an LCA according to the uncertainty framework developed in the "Confronting Uncertainty in LCA used for decision support" paper presented in the previous chapter. The paper also investigates a few options for optimized production and use of biodiesel based on different explanatory variables. The main part of this LCA study is on step 4 in the statistical value chain. However, it was not possible to strictly follow the procedures for step 1-3 in the statistical value chain and only a very limited control of the data mining in these steps has been possible. Some (unquantifiable) uncertainty in the LCA results should be expected.

The fifth chapter in the main text is based on the submitted paper: "**Comparative assessment of SimaPro and GaBi**". This paper compares the two commercial programs available worldwide (SimaPro and GaBi) on an equal basis, namely by entering the exact same LCA biodiesel case study into the two software programs. The study is based on the LCA type with the lowest possible inherent uncertainty according to the classification system outlined in "Confronting Uncertainty in LCA used for decision support" and the best possible AN available on the market – even then there is considerable uncertainty in the results according to the findings in this paper.

The sixth chapter in the main text is based on the submitted paper: "**Enabling optimization in LCA - from *ad hoc* to Structural LCA approach**". In this chapter, different types of optimization are enabled through what I have called the Structural LCA Approach. The optimization in this paper is done in a fair way since all the different pathways[2] are based on the same type of LCA study according to the classification system developed in the submitted "Confronting uncertainty in LCA for decision support" paper. This LCA used for decision support is on step 7 according to the statistical value chain.

Each of the chapters (3-6) which present the four papers that I have produced during this PhD project have been structured as a summary of the papers and each chapter contains three sections: "*The relation to the statistical value chain*", "*Further discussion*", and "*Value-adding*". Since the four submitted papers can be found in appendices "A-D", I have chosen to (only) present an executive summary of each paper in these chapters. These executive summaries are a more comprehensive description than the abstracts of the submitted manuscripts and emphasize details relevant to the common thread of this PhD thesis. In the section "The relation to the statistical value chain" it is highlighted how each paper relates to the statistical value chain. In the section "Further discussion" points and discussions that I would like to emphasize more than already done in the

[2] Each pathway is a *unique* solution in the LCA space.

papers (or have not presented at all but still see as relevant for the PhD thesis) are presented. Finally the section "Value-adding" emphasizes what each paper can contribute to the general LCA field.

The last chapter in this PhD thesis is "**Outlook and concluding remarks**". Five different topics are presented here: "The PhD project summarized into one equation", "How to keep track of all the changes in a long running LCA project used for decision support?", "Market effects in LCA used for decision support", "Do numbers used for decision support have a "supporting" capacity (limit)?", and "Expanding the idea of Hume's "is-ought" problem".

5 Methodologies and theory

The main approach for this PhD project has been through research of the literature. In the following the main areas, which I assume can be categorized as methods or methodologies and which I have used the most, are presented. A key guideline for this methodological outline is that our starting point is a *blank wall*, which is flat, and it is impossible to hang a hat or a jacket on the wall. The different methods and the concept outlined below can be thought of as *hooks* on the wall. With hooks we can hang hats or jackets on the wall – we can start to compile a narrative with a common frame of reference and articulate problems that have not been evident beforehand.

5.1 Hume – the "is-ought problem"

The *is-ought problem* was formulated by the Scottish philosopher David Hume in the book *A Treatise of Human Nature*. (Hume 1888) The is-ought problem reflects a fundamental problem of how we can deduce what we *ought* to do. Hume argues that no objective rule can be formulated with regard to what we ought to do. Assumptions about what we ought to do, or beliefs about what is good and what is bad, are fundamentally subjective as a result of infinity regress. In infinity regress "supporting argument A" is supported by "supporting argument B" which again is supported by "supporting argument C" etc. However, we can say that the state of the World *is* formed in a certain way both with regard to a strictly physical perception and with regard to a perception of how humanity is organized.

The is-ought problem is relevant for this PhD thesis. For example, if we know that the uncertainty of a specific LCA result *is* high (and potentially not even possible to quantify), what *ought* we to do then: should we use the result for decision support or not? In this PhD thesis the is-ought problem is used for the sake of reflection in the context of LCA usage for decision support.

5.2 Statistics and probability theory

Statistics deals with collecting, organizing, analyzing, and interpreting of data. It also deals with the planning of data collection in terms of the design of surveys and experiments. Hence statistics has a rather big application potential and relevance for LCA. Statistics has been used as a benchmark against the *de facto* data handling approach in LCA. Furthermore, the application of statistics in this PhD thesis is assumed to be related to the "*is*-issue" in Hume's is-ought problem. That is, statistics only provide facts if used correctly. On the other hand, whether to use statistics or not is an "*ought-*issue". Main references for this methodology are: Loève (1963); Cochran (1977); Pitman (1993); Gy (1998); Crawley (2005); Montgomery (2005a); Petersen, Minkkinen & Esbensen (2005).

5.3 Management and economic theory

Since the LCA methodology in general is thought of as being a decision support tool, it also has a rather large convergence with the management theory field especially decision making (and support) theory and economic theory. Two distinct schools of management theory are "the rational school" (as discussed in e.g. the book "Decision Making" (Lindley 1985)) and what I will in this PhD thesis refer to as the "Anarchistic school" (as discussed in e.g. the book "Decisions in organizations"/(Beslutninger i organisationer) (Enderud 2003)). The generalization of the management theory field into these two distinct schools might seem to be a gross oversimplification, but for this PhD thesis I see it is an acceptable distinction. In general the rational school is concerned with and develops "ideal models". For example, ideally we ought to base decisions on correct sampling procedures and statistical analyses. The anarchistic school is concerned with: "*what people really do and how they really make decisions*". For example, often people do not make decisions based on proper sampling and statistical analysis but rather on power relationships between people. Such power relationships can be both formal and informal relationships. Using this distinction of the management literature I would claim that the majority of this PhD thesis builds on methods, assumptions, and theories from the *rational* school. Decision making theory as outlined by Møller (1996), Lindeneg (1998) and Hanley, Shogren & White (2007), has served as a methodological foundation for this PhD project. For example, different types of decision making situations are analyzed in this literature, such as having one DM with one objective or having more than one DM with more than one objective. These decision making problems are *not* trivial. Two distinct management schools that also have been convenient to use in the context of LCA are the schools of "planned management" and the school of "adaptive management" (Collins 1998; Kotter 1999; Cummings & Worley 2001; Weick 2001; Johnson, Scholes & Whittington 2005; Morgan 2006). The relevance for LCA, used for decision support, based on these schools can be summarized as: "*given that we have a fixed amount of resources to make an LCA, what strategies do we choose between for using these resources*?"

5.4 LCA

In the following references to LCA literature is presented including a short description of content of the different references. These references have, among others, formed my platform of knowledge of what is the "current" situation of LCA. This literature does not stand alone for forming my "LCA knowledge platform" since much of my knowledge has come from many discussions with my supervisors and colleagues.

I have chosen to divide the literature into two categories: "LCA theory" and "applied studies". The "LCA theory" category has primarily been target towards "uncertainty LCA literature" and has a generic character, while the "applied studies" is target specifically to biofuels and especially biodiesel.

LCA theory (focusing on uncertainty)

Basic LCA methodology (i.e. "*how to conduct an LCA?*") is addressed in Wenzel, Hauschild & Alting (1997). In Wenzel (1998) it is pointed out that LCA can be application depended, i.e. "how to conduct an LCA" depends on the actual decision support context. This is very much also the stand-point of this PhD thesis. Huijbregts et al. (2001); Ross, Evans & Webber (2002); Huijbregts et al. (2003); Weidema et al. (2003); Ciroth, Fleischer & Steinbach (2004); Heijungs & Huijbregts (2004) have proposed different approaches for identifying and quantifying uncertainty in LCA. The general approach suggested in these articles is summarized in the three-step procedure below, which is basically an exercise in variance propagation:

- Collect data, (normally from the literature and often resulting in single point estimates)
- Estimate variation or uncertainty range for individual data (expert guesses or estimates, for example "+/-10 %" as suggested in (Huijbregts et al. 2001) or using the pedigree reliability matrix developed in (Weidema, Wesnæs 1996).
- Apply Monte Carlo or similar simulation tools to propagate variation ranges and model uncertainty.

Huijbregts (1998) observes that it may not be possible to actually quantify or reduce (model) uncertainty in LCA when it arises from lack of information. In a range of papers it is advocated that

LCA's should take a market orientated approach and such types of LCA is categorize as the "Consequential LCA approach" among these papers, and some reports, are: Weidema, Frees & Nielsen (1999); Weidema (2001); Weidema (2003); Ekvall & Weidema (2004); Ekvall & Andrae (2006). The main assumption in the Consequential LCA approach, as I understand it, is that an LCA should (*ought*) to describe (all) the consequence of a decision made or action taken. My concern here is that predicting all consequences of a decision made might sometime be an ambitions "project". I would consider such a project in relation to the resources available to the AN. This is an issue I have found relevant to consider and address in this PhD project. Weidema (2009) reflects on the possibilities of (intentional or unintentional) avoiding or ignoring uncertainty in LCA based on an "uncertainty-relevance"-diagram presented in Hauschild & Potting (2005). Ciroth (2006) describes what he calls the "missing link in LCA". The missing link is validation of the LCA results, that is: "*...you check whether the model you have built is correct by comparing it to the reality you attempted to model*". This I would assume is an important consideration which also is in alignment with "adaptive management principle". Hertwich, Hammitt & Pease (2000) gives what they call "A Theoretical Foundation for Life-Cycle Assessment" where they consider the role of values in environmental decision making. Mathiesen, Münster & Fruergaard (2009) indicates that it can be difficult or lead to uncertainty when attempting to identify "marginal production". Makridakis (1998), Bezdek & Wendling (2002), and Nielsen & Karlsson (2007) evaluates different forecast studies in relation to the energy market and finds that forecasting is a very difficult task and discuss the reliability of such forecasts. McKone et al. (2011) recognize that uncertainty is (still) a challenge for applied LCAs used for decision support.

Applied studies (focusing on biofuels)

Harding et al. (2008) develops a LCA of biodiesel production and compares enzymatic and conventional transesterfication process in a well-to-tank perspective with multiple impact categories. This study was to some extent the foundation of the first LCA developed in this PhD project. Malça & Freire (2011) present a comprehensive review of 28 different LCA studies on biodiesel in Europe where all results are evaluated based on green house gasses (GHG) emissions per MJ. The two main issues raised in this review study are the variability of results and the different modeling approaches between the different LCAs. According to Howarth et al. (2009) some, but few, biofuel studies reports on other environmental impacts than GHGs, for this reason I have addressed 6 different impact categories for the biodiesel study. Bernesson, Nilsson & Hansson

(2004) gives what they call "A limited LCA comparing large- and small-scale production of rape methyl ester (RME) under Swedish conditions" study. It is shown in this study that the differences in environmental impact and energy requirement between the small-, medium- and large-scale systems were small or even negligible. However, also different allocation types were used: *physical allocation, economic allocation, no allocation, and expanded system*. The results were largely depending on the method used for allocation of the environmental burden between the RME and the by-products meal and glycerine. Edwards et al. (2007); Dalgaard et al. (2008); Searchinger et al. (2008); Hedal, Baltzer & Nielsen (2010); Schmidt (2010); all gives "consequential" modeling approaches (or expectations of what might happen in the future) regarding different agricultural systems. Nielsen, Oxenboll & Wenzel (2007) makes a cradle to gate LCA of enzyme production. Halleux et al. (2008) makes a comparative LCA of ethanol from sugar beet and rapeseed methyl ester. "The biodiesel handbook" by Knothe, Krahl & Van Gerpen (2009) I assume is "the book" regarding biodiesel production presenting many relevant technical relevant details/options for biodiesel production and some market information (although they might be outdated by now). Sotoft et al. (2010) gives a process simulation (and economical evaluation) of enzymatic biodiesel production plant. Sander & Murthy (2010) gives a retrospective baseline study of biodiesel production with the purpose of benchmarking potential of other algae based biodiesel LCA studies. Almeida et al. (2011) benchmarks the environmental performance of a jatropha biodiesel system through a generic LCA. Sanz et al. (2011) presents a LCA of a biofuel production process from sunflower oil, rapeseed oil, and soybean oil. Varanda, Pinto & Martins (2011) gives an LCA of biodiesel production based on palm oils and waste cooking oil.

6 The statistical value chain

Most application-oriented LCAs are used as an "overall linkage" decision support tool, meaning that they summarize a relatively large amount of data mainly collected in the literature, e.g. articles, various databases and reports, which rarely give anything other than point estimates (such as an average value). Previous methods for evaluation of uncertainties in LCA have mainly been based on estimates from experts and variation expansion, for example by using Monte Carlo simulation. Papers like Ross, Evans & Webber (2002); Huijbregts et al. (2003); Ciroth, Fleischer & Steinbach (2004); Heijungs & Frischknecht (2005) address uncertainty in LCA and how to quantify this.

My suggestion for an improved approach to LCA is based on what I regard as the "*statistical value chain*" (presented below) which is partly derived from Gy (1998) and Petersen, Minkkinen & Esbensen (2005) but also more classical statistical and probability theory, such as Pitman (1993); Johnson (2005); Montgomery (2005a). Whether or not to (strictly) apply this statistical value chain is an "*ought problem*". If the AN (or the DM) has to be in control of the full statistical value chain it will unavoidably be a much more resource-intense procedure to perform LCAs than it is today. The value-adding part to LCA, used for decision support, might not necessarily come from a strictly rigid application of this statistical value chain. The value-adding part to LCA used for decision support can come from an understanding of the statistical value chain which can make it easier for the ANs and DMs to evaluate data and the data sampling procedures used for LCA which are used for decision support. Deviation from this statistical value chain will simply lead to an increased uncertainty in the LCA used for decision support.

It is not the goal of this PhD thesis to describe in detail the steps of the statistical value chain. Each step is described thoroughly in the literature and references will be provided to this literature.

The statistical value chain

I assume that it is a matter of *fact* how the world is at any given point in time (P_t). I also assume that the state of the physical world can be described as the location and quantity of matter and energy in time and space.

How the state of the world was at $P_{t-1\ \dots\ t-m}$ (retrospective) is unchangeable. Based on the rational school of management, I assume that prospectively ($P_{t+1 \dots\ t+n}$) it is possible to influence the state of the world. However, it is necessary that stringent rules for induction, deduction, and abduction are applied to get the clearest picture of the state of the world and to understand how we can affect this state to be in a more desirable state (at a later point in time). Statistics is the (applied) science of deduction (and induction). For this reason I have assumed that statistics can be an acceptable benchmark point for LCA used for decision support.

Initially, I will distinguish between 1) a *physical world* which is the location and quantity of matter and energy in time and space, and 2) *value* - which is the value placed on that same physical entity by one or more DMs. In the following statistical value chain, steps 1-7 are only concerned with the physical properties of the world.

Step 1: Defining the population(s) that is/are desired to be investigated.

For information about the world (given in step 1), we need to collect empirical data. Obviously we cannot collect data on the entire world, but we need to collect data on the population(s) that we are making inquiries into. The starting point of data collecting procedure is to *define* (or outline) the population(s) which we want to make inquiries into, both with regard to space and time, e.g. a specific corn field at present (year 2012), all soybean fields in a given country (year 2006), or a batch of print circuit boards (year 2014). In most LCAs there are normally many populations to collect data from, which I will refer to as a product *system*.

Step 2: Full investigation or Theory of Sampling (TOS).

When we have defined the product system that we want to make inquiries into, then we have two options for seeking information about this or these population(s): A) seek full information (i.e., examine all populations in the entire product system or B) using representative sampling for each population in the product system. The latter method (TOS) is one of the statistical methods that, in principle, are designed to conserve resources compared to the first procedure where all populations have to be investigated fully in the product system (Cochran 1977). Only well-used sampling procedures described by TOS can lead to representative sampling of the different populations in the product system. The starting point of any sample procedure is outlined in step 1. The sample size, and hence resources needed, depends on: 1) how accurate does the DM need the results to be? 2) the population size, and 3) the true variation of the population. To gain representativeness (unbiasedness and accuracy), it is important that all items of the population are *randomly* chosen, meaning that they have equal probability of being sampled. For example sampling from a batch of print circuit boards, in (e.g. four) containers, it is not a correct sample procedure to pick the 10 circuit boards closest to the container door(s). One correct procedure for sampling from such a batch of print circuit boards can be to label all the print circuit boards with consecutive numbers and then use a program to draw randomly between these numbers. Correct sampling is not a trivial task and according to Gy (1998) and Petersen, Minkkinen & Esbensen (2005) there can be grave errors in applied sampling. As noted by Petersen, Minkkinen & Esbensen (2005), using incorrect sampling procedures in the sampling process will potentially corrupt the rest of the statistical value chain used for decision support: "*Without representativity in this first stage in the entire analytical chain, there is no way of ever evaluating the degree of sampling bias and sampling errors embedded in the final analytical results subjected to data analysis. It has been known for more than 50 years that the combined sampling errors typically amount to 10–100, or even as much as 100–1000 times the specific analytical errors*".

Step 3: Descriptive statistics.

Descriptive statistics is about computing averages, variation analysis, min and max, distributions, confidence intervals, etc. for each population investigated. See Johnson (2005) for further information on this step. This step is to some degree trivial and the quality of this step is closely linked to the AN's capability to undertake these computations (Gy 1998).

Step 4: The retrospective LCA.

Abraham Lincoln once said: "*Prior to determining where we are going: we must first ascertain from whence we came*" (quoted from (Bezdek, Wendling 2002))

As long as a given LCA can be categorized as a *retrospective* assessment I assume that LCA is a matter of accounting and based on the previous steps this accounting is, more or less, straight forward and the accounting should cover the total LCA system, i.e. all populations. This is analogous to a company's financial statement. In Gowthorpe (2003) and Andersen, Rohde & Worre (2005), the problems of-, how to make-, and basic assumptions of financial statement are described. I assume that the better (more accurate and unbiased) the accounting has been done, the better it can serve as a *starting point* for *prospective* LCA assessments. I also assume that the better the AN is equipped to investigate the retrospective LCA, the better the AN can provide prospective LCAs –

analogous to issues treated in "*Financial statement analysis*" (Wild 2007). "PWA1"[3] in the submitted paper "Potentials for optimized production and use of biodiesel in a well-to-wheel study" (Appendix B) is a retrospective assessment of biodiesel.

Step 5: Developing the baseline for prospective LCA.

The first step in prospective assessment is to construct a baseline, which should be characterized by: "*exactly what (you think) will happen if the change under consideration was not introduced*". The following step (step 6) outlines methods for the prospective LCA.

Step 6: The prospective LCA – based on inferential statistics.

To make a *prospective* LCA, a "(LCA-)model for forecasting" is needed where information and data gathered in the past (retrospective) can be used for forecasting and prediction.

1. "*Naïve forecast method*": The simplest method to make a forecast into the future is to use the "*naïve forecast method*" (Makridakis 1998), which assumes that the best forecast for the future is the current value (of a given time series). However, in many cases it is unlikely that a product system will remain *static* over a longer time period, and sometimes even a shorter time period. Hence, using the naïve forecast method can lead to inaccuracy and bias (compared to methods described below). Different *forces* can affect the product system. Such forces, I will initially assume, can be divided into *exogenous* forces and *endogenous* forces. Exogenous forces are forces that the DM cannot (or at least not easily) influence - they are imposed from "the outside". Endogenous forces are controlled by the DM by making different alterations to the product system.
2. "*Times series*": How exogenous forces and endogenous forces can impact the product system might be possible to deduce by studying *time series*, given that time series have been adopted for both the product system *and* the forces that might impact the product system. Based on this information about the different forces that can affect the system, we can attempt to make forecasts and trend analysis (Makridakis 1998). However, the study of time series can be dangerously misleading. As an example, maybe 10 different exogenous forces might affect a product system, but 5 of these forces are unknown to the AN, and only two of the "known forces" have reliable times series available. If the AN makes a correlation

[3] PWA1 = pathway for producing and using biodiesel based on rapeseed and petrochemical methanol feedstock based on present conditions.

analysis based on a response variables for the product system and the (available) time series for the two known exogenous forces affecting the production system and base a forecast on this correlation factor, the forecast might be biased and misleading. Also, an observed correlation between different time series does not necessarily indicate that there is a causality relation. Only sound human being judgment can be used to tell whether there is a causality relationship or not. Information on the different forces affecting a product system might (in many cases) already be summarized and made available through the literature (and other places). Given that this is the case, we do not (necessarily) need to make time series studies ourselves to investigate the impact of different forces on the product system. This is to have a prior knowledge of the forces. In the following I will use “explanatory variables” interchangeably with “forces”. As an example, take the endogenous explanatory variable “alcohol type” in the product system modeled in the submitted paper “Enabling optimization in LCA from *ad hoc* to Structural LCA approach” (appendix D). For this endogenous explanatory variable (or force), information (stoichiometry) was already available in the literature, which was used to assess how this explanatory variable/force can impact the response variables for the product system/FU.

3. *Explanatory model*: Through the use of explanatory models we can (also) produce forecasts (Montgomery 2005a). These models consist of explanatory variables and response variables. In the submitted paper “Potentials for optimized production of biodiesel in a well-to-wheel study”, this method is applied. A breakdown of the explanatory variables can be useful for improvement of the forecasting. The following breakdown of the explanatory variables is not necessarily a complete list of possibilities, rather it is a suggestion for what at least can be considered as a starting point:
    a. The explanatory variables can be separated into the four categories which can be referred to as the “(un)knowns”: “*The known knowns, the known unknowns, the unknown knowns, and the unknown unknowns*” (as articulated by the former US Secretary of Defence, Donald Rumsfeld)[4]. This distinction of different explanatory variables is partly also reflected in Walker et al. (2003) and Montgomery (2005a), which outline an uncertainty continuum going from “statistical uncertainty” to “total ignorance”. See Walker et al. (2003) for further information.

[4] I have made no attempt to track where this quote originally is from.

b. Both endogenous and exogenous explanatory variables can affect a system. It is important to consider both types of explanatory variables when defining the baseline while forecasting.

c. The PESTEL framework Johnson, Scholes & Whittington (2005) can be used as a further breakdown of the explanatory variables. PESTEL is an abbreviation for: Political-, Economic-, Sociocultural-, Technological-, Environmental-, and Legal-explanatory variables. For further information of the PESTEL framework see Johnson, Scholes & Whittington (2005).

One of the most important factors when forecasting for decision support is that the explanatory variables are adjusted correctly and those that explain environmental impact from an investigated product system are *not* missed. If explanatory variables that explain environmental impacts from a product system are missed then it can result in bias or too much "weight" on the applied explanatory variables. For example, it can be misleading when land use changes are explained, more or less, as being driven solely by the increased production of biofuels in other countries as seems to be the case in papers like Searchinger et al. (2008) and Schmidt (2010). Some explanatory variables can also change drastically over time (i.e. the coefficient used for characterizing a given explanatory variable); for example, "land use change" may vary from year to year depending on political processes, which can be hard to predict. On the other hand, it seems impossible to include all explanatory variables or forces affecting the product system. Hence, the model constructed for forecasting will be inadequate given that the DM expects a model that explains "everything" or at least expects *more* than the model actually accounts for. This is uncertainty that I would claim originates from obscurity. This is discussed further in subsection "Further discussion. Transparency: Confronting *obscurity* in LCA used for decision support" in the chapter "Summary - Confronting uncertainty in LCA used for decision support.

Step 7: Alternatives.

All relevant alternatives to the baseline study developed in step 5. The difference between the baseline study and alternatives provides the potential for change (both positive and negative).

Step 8: Valuation.

As mentioned before, in steps 1-7 I have only been concerned with strictly physical properties of the world. In step 8 "valuation" is considered. Valuation in this PhD thesis is understood as the *process* of placing a value on the physical entity by one or more DMs treated in step 1-7 above. I assume in this PhD thesis that valuation is fundamentally a process happening in collaboration with all DMs in a society that is democratic and applies to an Arrow-Debreu economy[5] (Lindeneg 1998). Furthermore, in the following it is assumed that these entities can be both tangible and intangible. Broadly, in the following section I will refer to these tangible and intangible entities as goods. It seems to me that the valuation of goods and how this step should be approached is an *ought*-issue. It is beyond the scope of this PhD to compare different methods to assign values to these goods. However, by shortly describing three problems (points I, II, and III below) recognized in the economic literature regarding valuation of goods, this should indicate why valuation from an economic perspective is *not* trivial and why this step can lead to increased uncertainty if this step is included in an LCA used for decision support.

The starting point of valuation from an economical perspective is an Arrow-Debreu economy where no market failures takes place and as a result of this resources/goods are allocated in a Pareto Optimal (PO) way. Pareto optimality means that resources are allocated in such a way that it is not possible to reallocate the resources in a way where someone is better off without someone else being worse off. (Lindeneg 1998)

I. When a transaction in an Arrow-Debreu economy takes place then a price is established on a good, and this gives the real price of the good. Before this transaction takes place (and potentially afterwards) the owner (or any agent in the market) might, for strategic reasons, claim that the good is worth much more to the owner (or other agents in the market) than it actually was traded for (Lindeneg 1998; Johnson, Scholes & Whittington 2005). Values on goods not adopted from actual transactions have a firm risk of being biased.

II. Environmental problems can be considered as being transactions that do not happen on a market and especially not in an Arrow-Debreu market. These transactions fall victim to market failures (Hanley, Shogren & White 2007). I will broadly refer to these transactions as being *externalities*. Methods to determine valuation of goods when the values are not adopted directly from a market in an Arrow-Debreu economy are many, but the odds that these methods are inaccurate and biased are high.

[5] An economy without market failures.

III. Values placed on different physical entities change constantly over time. If such changes are not reflected when the value of a particular good is given, then it also can lead to increased uncertainty and biases.

Based on these findings, I find it reasonable to assume that valuations that are not adopted from a perfect market are 1) resource-intensive, and 2) can potentially lead to rather large bias and hence to incorrect decision support. Cost-Benefit-Analysis (CBA) can be used to assess the value of a given project when the market fails. Different methods for making CBA are available, such as: Avoided-Cost-Analysis, Social-Cost-Benefit-Analysis (SCBA), Cost-effectiveness analysis (CEA), Scoring-methods, Willingness-To-Pay (WTP) analysis, Willingness-To-Accept-Compensation (WTAC) analysis etc. For further information see Møller (1996); Lindeneg (1998); Hanley, Shogren & White (2007). In a specific LCA context, valuation has been treated and discussed in Volkwein & Klöpffer (1996); Volkwein, Gihr & Klöpffer (1996); Wenzel, Hauschild & Alting (1997); Hertwich, Hammitt & Pease (2000); Hauschild (2005); Finnveden et al. (2009). It is beyond the scope of this PhD thesis to elaborate further on valuation in the context of LCA.

Additional remarks concerning the statistical value chain.

An AN (and DM) faces two challenges when collecting data for LCAs used for decision support:

1. That the uncertainty (accuracy and bias) level of the LCA results delivered from the AN to the DM is not in alignment with the DMs accepted uncertainty level due to *incorrect* data collection procedures, i.e. by not following the above described procedure or by using smaller samples than announced.
2. If the AN has not been in control of the entire value chain, then the data could potentially be corrupted due to *strategic* behavior from other agents in the market delivering the supporting data as it is a well-known phenomenon that agents act strategically (Lindeneg 1998).

The statistical value chain should not necessarily be thought of, or used as, a rigid procedure for using statistics in LCA for decision support. As it is recognized in Collins (1998), projects can rarely be put on a chain with a certain and correctly defined numbers of steps before the project end is reached. How a project develops is often better described as being an *ex-ante* "*N*-step" process, meaning that a project is an iterative process with a previously unknown number of *N*-steps, going back and forth between the different steps.

Whether to use or not to use the statistical value chain is, as mentioned, an "*ought* problem" and hence no formal or objective rules can be deduced for using the statistical value chain. One major challenge for the statistical value chain is that it is cost-intensive. However, both Gy (1998) and Petersen, Minkkinen & Esbensen (2005) argue that (at least in the long run) it will pay-off to use proper sampling techniques, and hence also using the rest of the statistical value chain. On the other hand, it can be argued that if the DM pays little attention to LCA results/decision support in a decision making process then it might not be worth spending too many resources on the LCA decision support since a high uncertainty in the LCA results will not make much of a difference.

7 Executive summaries of papers produced in this PhD project

In the following four subchapters executives summaries for the four papers that I have submitted are presented. These papers can be read in their entirety in the appendix section:

A) Confronting uncertainty in LCA used for decision support - Developing a Taxonomy for LCA Studies (**Appendix A**) (Herrmann et al. 2012a)
B) Potentials for optimized production of biodiesel in a well-to-wheel study (**Appendix B**) (Herrmann et al. 2012c)
C) Does it matter which LCA tool you choose? - (**Appendix C**) (Herrmann et al. 2012b)
D) Comparative assessment of SimaPro and GaBi on a biodiesel case study (**Appendix D**) (Herrmann et al. 2012d)

7.1 Confronting uncertainty in LCA used for decision support

- ***Developing a Taxonomy for LCA Studies***

The goal of this paper is to present a taxonomy of terms used to explain and classify the types of uncertainty one faces in a typical Life Cycle Assessment (LCA). The hope is that the taxonomy will provide life cycle analysts, decision makers, and stakeholders with a common language to describe both the certainty and ambiguity of LCAs and will therefore improve the effective interpretation and application of LCA results. LCA offers a quantitative approach to assessing environmental impacts from products, technologies, and services. LCAs are conducted by LCA practitioners or analysts to help DMs map the tradespace between various competing attributes, which may include protection of near- or far-field environmental quality, maximizing economic benefits, and improving production timelines. At present, some DMs may have reservations about the LCA process as a reliable decision support tool. One cause is the perceived crude manner with which uncertainty is incorporated into typical LCAs, or the sometimes wide uncertainties reported in the LCA literature. Many researchers are developing algorithms and processes to better quantify and compute uncertainty in end results. In this paper, we provide a higher level explanation of the various forms of uncertainty in a typical LCA. The resulting taxonomy will improve how future LCA analysts and DMs interpret results and rank the relative importance of various uncertainties.

The taxonomy has been developed through comprehensive studies of the LCA literature with inspiration from the management literature, as well as the economic literature. The taxonomy is presented in Table 1 below.

Table 1. Dimensions used to classify LCA studies.

Tangibility **Tangible (T) vs. Intangible (I)**	Tangible things can be measured and touched in the corporeal world. In contrast, intangible things can be ideas or concepts. Only hypotheses and indirect evidence can be made about intangible things.
Time **Retrospective (R) vs. Prospective (P)**	Retrospective studies deal with what happened in the past while prospective studies involve estimation of future events.
Repetitivity **Single-period (S) vs. Multi-period (M)**	A single-period is, for example, the CO_2 emissions from a given factory in 2008. A multi-period is for more than one year, say the CO_2 emissions from a given factory in 2007, 2008, and 2009.
Change **Baseline (B) vs. Change (C)**	The baseline is business as usual while a change is any deviation from the baseline.
Scale **Micro (i) vs. Macro (a)**	In a relative size scale, micro is small compared to macro, but the absolute scale depends on what is relevant for the studied function or service.
Value **Physical (Y) vs. Value (V)**	Physical refers to the location and quantity of matter and energy in time and space. Value refers to the value placed on that same physical entity by one or more DMs.

In the paper, this taxonomy is related to the probability principle known as the Law of Large Numbers (LLN). The LLN is here interpreted as: "*the larger a sample (n) from a given population is, the more accurate the estimate of the true average of the population (N) will be*". Furthermore, I have assumed that *N* can be interpreted as the LCA *space* about which we are making LCA statements. An LCA statement is the answer to an LCA question (or inquiry). For more information about the LLN see (Loève 1963) or (Pitman 1993). This relation is illustrated by the pedigree matrix provided in Figure 1, as presented on the following page.

			Tangible (T)				**(Tangible +) Intangible (I)**			
			Single-period (S)		**Multi-period (M)**		**Single-period (S)**		**Multi-period (M)**	
			Micro (i)	**Macro (a)**	**Micro (i)**	**Macro (a)**	**Micro (i)**	**Macro (a)**	**Micro (i)**	**Macro (a)**
Retrospective (R)	**Baseline (B)**	**Physical (Y)**	TSi-RBY	TSa-RBY	TMi-RBY	TMa-RBY	ISi-RBY	ISa-RBY	IMi-RBY	IMa-RBY
		Value (V)	TSi-RBV	TSa-RBV	TMi-RBV	TMa-RBV	ISi-RBV	ISa-RBV	IMi-RBV	IMa-RBV
	Change (C)	**Physical (Y)**	TSi-RCY	TSa-RCY	TMi-RCY	TMa-RCY	ISi-RCY	ISa-RCY	IMi-RCY	IMa-RCY
		Value (V)	TSi-RCV	TSa-RCV	TMi-RCV	TMa-RCV	ISi-RCV	ISa-RCV	IMi-RCV	IMa-RCV
Prospective (P)	**Baseline (B)**	**Physical (Y)**	TSi-PBY	TSa-PBY	TMi-PBY	TMa-PBY	ISi-PBY	ISa-PBY	IMi-PBY	IMa-PBY
		Value (V)	TSi-PBV	TSa-PBV	TMi-PBV	TMa-PBV	ISi-PBV	ISa-PBV	IMi-PBV	IMa-PBV
	Change (C)	**Physical (Y)**	TSi-PCY	TSa-PCY	TMi-PCY	TMa-PCY	ISi-PCY	ISa-PCY	IMi-PCY	IMa-PCY
		Value (V)	TSi-PCV	TSa-PCV	TMi-PCV	TMa-PCV	ISi-PCV	ISa-PCV	IMi-PCV	IMa-PCV

Figure 1. Pedigree matrix for LCA studies showing the 64 different types of LCAs with corresponding inherent uncertainty, when keeping the resources constant for the AN. Moving from the upper left corner to the lower right corner, the expected uncertainty will increase. The index system can be used to describe which type of LCA question will hold the most uncertainty. The index system is formed from the abbreviation code for each dimension. For example if the LCA question involves tangible, multi-period, micro, retrospective, changes, and physical, then the index code for this LCA problem is: TMi-RCY.

The relation to the statistical value chain and LCA used for decision support

The pedigree matrix can be interpreted as a *mirror* of the statistical value chain; however, the steps 1, 2, and 3 are not explicitly expressed in the pedigree matrix. Steps 1, 2, and 3 are assumed to be prerequisites for developing any type of LCA.

If we use the "is-ought" problem, then the pedigree matrix illustrates the "*is*-issue" of how uncertainty will increase as we attempt to be more all-embracing whilst keeping the AN's resources constant. This is *fact*. How to handle this problem is an "*ought*-problem" that depends highly on the decision support context. For example, different DMs can have different risk attitudes, and different applications can have different requirements to the uncertainty of the results which can influence the choice of LCA used for decision support. This is discussed further in the paper. Different ways to confront the uncertainty in LCAs can be to 1) decrease the size of the LCA space, 2) increase the resources for the AN, or 3) apply the statistical value chain when conducting LCAs (given that it is not already applied, or considered to be applied).

Further discussion. Transparency: Confronting obscurity in LCA used for decision support

To some degree, obscurity can be used interchangeable with uncertainty. However, in this PhD thesis I am using the word *uncertainty* in relation to what I consider to be covered by the rational management school while I am using the word *obscurity* in relation to what I consider to be covered by the anarchistic management school. For example, the word *obscurity* covers problems such as miscommunication and misinterpretation of LCA results.

Transparency is important in a decision making context. The less transparent the LCA information is, the more time and resources the AN has to use to deliver the LCA results to the DM and to explain general assumptions, LCA specific assumptions, calculation methods, etc. As the name Life Cycle Assessment implies, LCA is a methodology that aspires to be all-embracing. Especially in recent years, with the introduction of consequential LCA (CLCA), (such as: Ekvall & Weidema (2004); Lund et al. (2010); Thomassen et al. (2008)), this aspiration has been even more expressed. Whilst it would be optimal to be able to predict all the consequences of our decisions, it is simply not a realistic option. As can be seen from the pedigree matrix as the size of the LCA space is increased the the LCA becomes more uncertain when keeping the resources for the AN constant. There will always be a trade-off between how uncertain the assessment will be and how all-embracing it is.

From my early research in the literature on the LCA of biodiesel it became clear that different LCA studies often arrived at different results for what seemed to be more or less the same product. This issue has recently been addressed in Malça & Freire (2011). Much of this observed variation in different LCA studies, I would claim, is not necessarily due to ill-made LCAs rather than due to widely different *foci* from different LCA experts and practitioners. The different foci are reflected in the developed taxonomy: six different dimensions with two extremes gives 2^6 (64) different combinations, all of which are presented in the pedigree matrix[6]. With this pedigree matrix it becomes possible to clearly state what is included in the given LCA and what is excluded.

By *articulating* (putting hooks on the wall) the different types of LCAs, we can make decision support more transparent and, to some extent, avoid obscurity in the LCA decision support. Knowing (exactly) what has been *excluded* from an LCA will also lead to increased transparency in an LCA used for decision support. In the economic literature the expression "*ceteris paribus*" is used to signify "all other things being equal" and we can think of the use of the pedigree matrix in a similar way when, for example, stating that the LCA is "only" a TSa-RCY LCA. Using this type of LCA does not mean that nothing else will happen prospectively.

As an example, Searchinger et al. (2008) suggests that corn-based ethanol will double greenhouse gases over the next 30 years and increase greenhouses gases over the next 167 years. This does not mean that there will be no effect on greenhouse gases by producing corn-based ethanol *after* the 167 years (from 2008) – it only means that Searchinger et al. (2008) *refrains* from predicting consequences, in terms of greenhouse gases emission, from corn-based ethanol more than 167 years into the future. From the information available in the Searchinger et al. (2008) paper I suggest it should be classified as an IMa-PBY LCA, which according to the pedigree matrix is one of the more uncertain types of LCAs used for decision support.

<u>*Value-adding*</u>

By using the developed taxonomy and pedigree matrix system as switches to clearly state what is included and what is not included in the LCA, a more transparent LCA can be delivered to the DM and hence this will reduce obscurity, uncertainty, time, and costs in the LCA used for decision support. By relating the LLN to the pedigree matrix it is also possible to rank the different types of LCA used for decision support on a scale of inherent uncertainty giving DMs, ANs, and other

[6] Some of these combinations are represented more frequently in the literature than other combinations.

stakeholders' important insight into the relative inherent uncertainty of different types of LCAs used for decision.

7.2 Potentials for optimized production of biodiesel in a well-to-wheel study

The increasing awareness of environmental impacts from petrochemical (PC) oil products (including PC diesel), the continuously increasing price, and the depletion of PC oil are all reasons for the increased focus on alternative fuels, such as biodiesel. For this reason, the European Union has enacted a proposal that requires each member state to ensure that the share of energy from renewable sources in transport in 2020 is at least 10% of final consumption of energy (The European Parliament and the Council 2009). This LCA study assesses the environmental impacts arising from the production and use of biodiesel as it is today (real-time), based on rapeseed oil and different types of alcohols using technologies that are currently, or are close to becoming, available. Different options for environmental improvement of production methods are evaluated.

The functional unit in this study is “1000 km transportation with a standard passenger car”. All relevant process stages have been included, such as rapeseed production (including carbon sequestration and N_2O balances) and transportation of products used in the LCA. System expansion has been used to handle allocation issues. In Table 2 below, eight different biodiesel pathways (PWs) and one petrochemical PW are presented. PWA1 and PWD0 are present conditions while PW2-PW8 are prospective PWs. Figure 2-7 presents the results for the nine different PWs.

Table 2 shows the different pathways for biodiesel production and use that are discussed in this paper. *PW = pathways, D = PC diesel, A = rapeseed,* and each ID-number is used to identify the unique combination. PWD0 and PWA1 are both considered as real baselines because they are today's real production and use. I = 0 t/(ha*year), II = 0.52 t/(ha*year), and III = 0.86 t/(ha*year).

	Biodiesel production step			
Name	**Alcohol production**	**Transesterification**	**Agriculture**	**Transport**
PWD0	No	No	I	No
PWA1	PC Methanol	Conventional	II	Short
PWA2	Bioethanol	Conventional	II	Short
PWA3	Bioethanol	Enzymatic 1	II	Short
PWA4	PC Methanol	Enzymatic 2	II	Short
PWA5	PC Ethanol	Conventional	II	Short
PWA6	PC Methanol	Conventional	III	Short
PWA7	PC Methanol	Conventional	I	Short
PWA8	PC Methanol	Conventional	I	Long

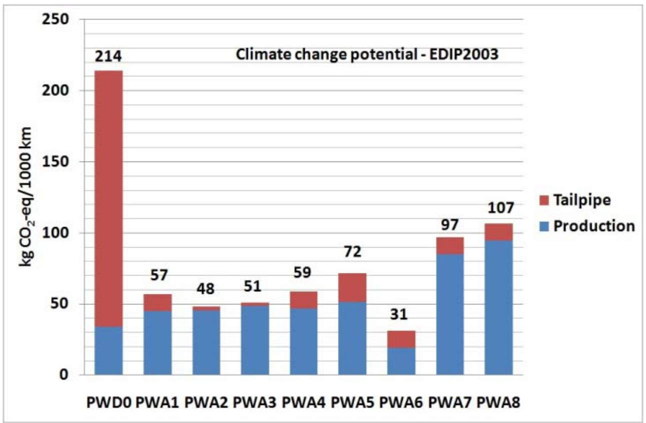

Figure 2. Climate change potential per 1000 km driven in a standard diesel passenger car - EDIP2003.

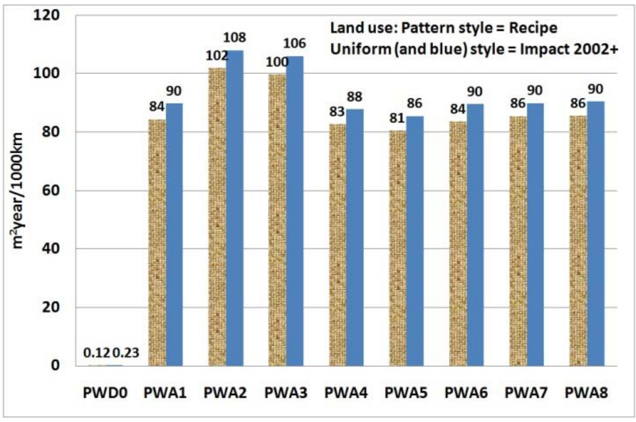

Figure 3. Land use based on Impact 2002+ and Recipe.

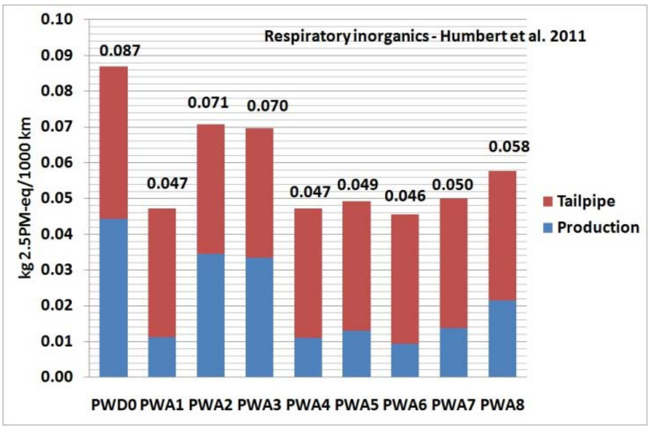

Figure 4. Respiratory inorganics - (Humbert et al. 2011)

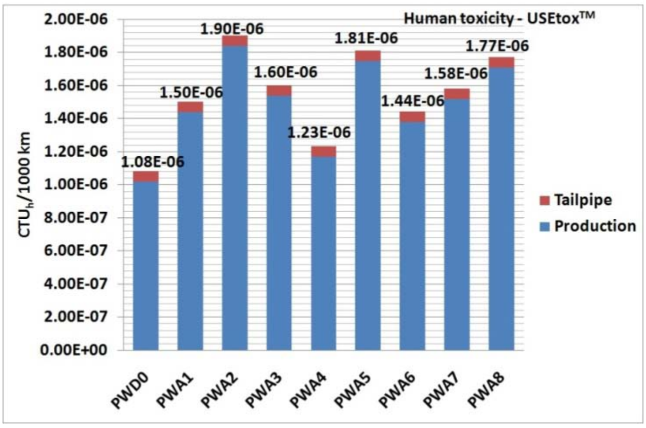

Figure 5. Human toxicity - USEtox^{TM}. CTU_h = comparative toxic unit, human.

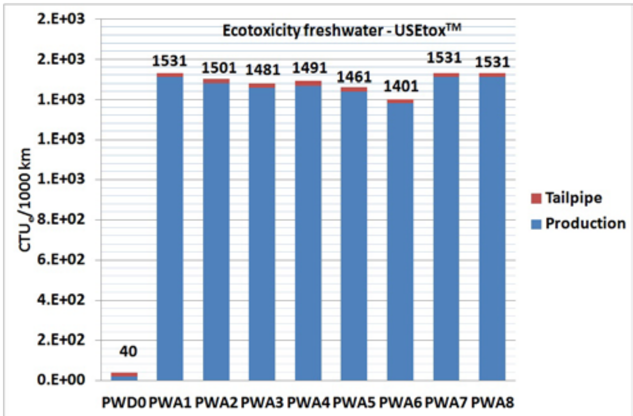

Figure 7. Ecotoxicity freshwater by USEtox^{TM}.

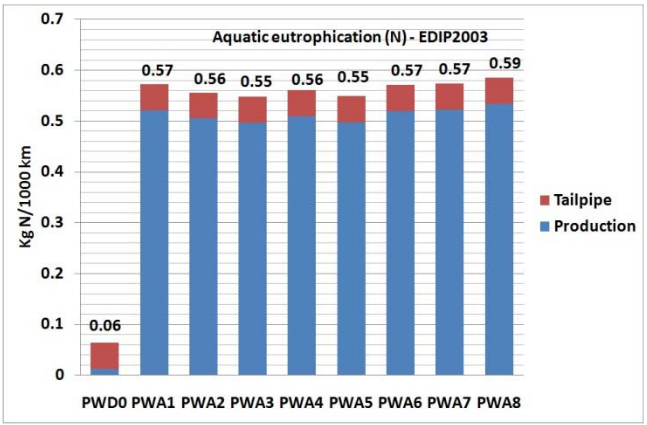

Figure 6. Aquatic eutrophication (N) using EDIP2003.

The following impact assessments have been used.

1. Climate change potential based on EDIP 2003 (Wenzel, Hauschild & Alting 1997)
2. Land use based on Recipe (Goedkoop et al. 2008) and Impact 2002+ (Jolliet et al. 2003)
3. Respiratory inorganics based on (Humbert et al. 2011)
4. Human toxicity (carc) based on USEtox™ (Rosenbaum et al. 2008)
5. Ecotoxicity freshwater based on USEtox™ (Rosenbaum et al. 2008)
6. Aquatic eutrophication (N) based on EDIP2003 (Wenzel, Hauschild & Alting 1997)

Six different impact categories have been evaluated in this study from a WTW perspective. The main sources of the environmental impact are summarized below and options for improvements are suggested.

In PWD0, the main source for climate change potential originates from the tailpipe emission with a tailpipe/(production + tailpipe)-ratio of 180/214 kg CO_2-eq./1000 km (~84 %). The impact from PWD0 is used to benchmark the findings for PWA1-8.

Climate change potential: For the different biodiesel pathways, the main impact comes from the agricultural stage where the use of mineral fertilizer (ammonium nitrate), traction for harvesting, and transport of rapeseeds especially contribute to the climate change potential. Potential for significant improvements in this production system comes from increased use of rapeseed straws for incineration (which is an assumed to substitute for coal) and lower transportation within the product system. Bioethanol or biomethanol can be used to reduce the tailpipe emission compared to PC ethanol or methanol.

Land use: PWD0 represents an insignificant use of land compared to PWA1-8. Using bioethanol compared to PC ethanol (or methanol) will increase the land use ~15-20 %. If it is desirable to decrease land use, then PC alcohol (and/or oil) is favorable.

Respiratory inorganics potential: PWD0 has the largest respiratory inorganics impact potential. Among PWA1-8, PWA2+3 have the highest impacts due to the use of bioethanol.

Human toxicity (carc) potential: The lowest impact is from PWD0. Between the different PWA1-8 there is some variation. The main sources originate from the production stage for both the PC diesel and the biodiesel. For PWA1-8, the largest contribution comes from the use of fertilizer. It is not preferable to change alcohol from PC methanol to bioethanol due to the increased human toxicity potential.

Ecotoxicity – freshwater potential: The PWD0 has, by far, the lowest impact. PWA1-8 have more or less similar impacts. Almost all of the impacts arise during the production system. The origin of this impact comes, almost entirely, from the use of pesticides in the rapeseed production.

Aquatic eutrophication (N) potential: The major difference in the aquatic eutrophication impact observed between PWD0 and PWA1-8 is due to the difference in the production system. Small changes between the different PWA1-8 can be observed. The origin of this impact comes mainly from the rapeseed production system with contributing parts from traction and the use of fertilizers.

The relation to the statistical value chain and LCA used for decision support

The two PWs PWD0 and PWA1 are on step 4 in the statistical value chain. However, it has not been possible to follow the statistical value chain for steps 1 to 3 in a stringent way so as to reduce the risk of bias and inaccuracy in this LCA used for decision support. I have, as the AN, had no control over the basic steps in the data collection procedure as outlined in the statistical value chain in this LCA study of biodiesel from a WTW perspective. Much of the data are from the Ecoinvent database (Faist, Heck & Jungbluth 2007), some data are from producers, while the rest of the data are from the general literature and hence it is not possible to know whether suitable randomization procedures have been applied when these data have been collected. This methodological uncertainty means that results can be biased, inaccurate, and obscure. On the other hand, it seems more or less impossible to protect an LCA against this risk due to the all-embracing nature of LCAs used for decision support since it would be exceedingly resource demanding to be in control of the entire statistical value chain. I have, throughout the project period, had the statistical value chain in mind and as such I do not think much more could have been done to reduce the uncertainty in the present LCA. PWA1 and PWD0 are, according to the pedigree matrix classified as one of the least uncertain LCAs used for decision support, namely ISi-RBY LCAs. The forecasting of all of the PWs has been done using the "*Naïve forecast method*" (Makridakis 1998).

Further discussion

To protect this LCA study of biodiesel from a WTW perspective against further bias and inaccuracy in the forecasting, the forecasting period was assumed to be short to avoid impacts from exogenous factors (known as well as unknown) on both the baseline studies (PWD0 and PWA1) and the alternative PW2-8. I assume that the forecasting period can be formulated in the following way: $P_{(t+1)}–P_{(0)} \rightarrow 0$, where $P_{(t+1)}$ is the next time-period and $P_{(0)}$ is the present time-period. This assumption also implies that it will be the DM that will bear the responsibility and risk if the conclusion of this paper is generalized to a greater account than this assumption allows.

Value-adding

The value-adding element of this paper, I would propose, is that it is one of the most stringent LCA studies, to date, performed on biodiesel from a WTW perspective. Uncertainty, bias, inaccuracy, and obscurity are reduced as much as possible. Furthermore, results for climate change potential, land use, respiratory inorganics potential, human toxicity (carc) potential, ecotoxicity (freshwater) potential, and aquatic eutrophication (N) potential have been evaluated.

7.3 Does it matter which LCA tool you choose?

- ***Comparative assessment of SimaPro and GaBi on a biodiesel case study***

SimaPro and GaBi are two of the frequently used software tools for LCAs. In this paper, their performance is compared based on an applied case study of biodiesel and some selected unit processes. The research question is: is there a difference between using SimaPro and GaBi, which influences the results and conclusions of the LCA study and the decisions based on it?

The performance of the two programs is compared following a 4 step approach:

1) Comparison of inventories obtained from GaBi (pe-international.com 2012) and SimaPro (pre.nl 2012) based on an identical biodiesel product system.
2) Investigation of some of the differences observed between SimaPro and GaBi in the first step.
3) Comparison of a standard unit process (i.e. "off-the-shelf" EcoInvent unit process) that has identical inventory in SimaPro and GaBi. Comparison performed at the level of characterization, normalization, and weighting using three LCIA methodologies, EDIP2003, CML 2001, and Eco-indicator 99.
4) Comparison of aggregated impact potentials obtained for the biodiesel product system.

A clear difference is observed for the inventories calculated for the biodiesel product system with SimaPro and GaBi. A ratio between the obtained inventory results of a factor of 10 is observed for the air-borne emission of 2,3,7,8-TCDD (dioxin). Most of the inventory differences observed are caused by differences in the way that the two softwares implement a single EcoInvent unit process on hydrochloric acid. Comparing the inventories obtained from SimaPro and GaBi for this process results in a maximum ratio of a factor 1380 for individual elementary flows. Also the implementation of the impact assessment methodologies shows considerable differences. For the same life cycle inventory, the maximum ratio for the characterized scores is 1160 for abiotic depletion calculated with the CML 2001 methodology. Finally, for the aggregated impact potentials obtained for the biodiesel product system, the difference between SimaPro and GaBi was observed to be a factor of 12. The observed differences seem to come mainly from errors in applied databases for both inventory and impact assessment.

SimaPro and GaBi are used by many LCA practitioners worldwide as a decision support tool. If the differences in the results obtained when using one or the other of the programs are generalizable, then the implications of this paper are worrying. It is clearly in the interest of both software developers and LCA practitioners that the observed differences are addressed in the future development of LCA decision supporting tools, e.g. through ring tests comparing the tools.

The relation to the statistical value chain

This GaBi-SimaPro study builds on the PWA1 presented in the previous paper "Potentials for optimized production of biodiesel in a well-to-wheel study". The PWA1 is on "step 4". Compared to the later steps, this is a less uncertain step. This can also be seen from the pedigree matrix where this PW corresponds to a ISi-RBY LCA, which is one of the least uncertain LCA types.

Further discussion

The results from this paper indicate that even though I as the AN have done everything that I think is possible to reduce the uncertainty, bias, and inaccuracy in the performed LCA, then there is still some uncertainty involved in the LCA used for decision support. The uncertainty revealed in this paper must have arises somewhere in steps 1-3 of the statistical value chain.

Value-adding

The value-adding of this paper is that it brings to light the errors involved in the data collection procedure arising from the use of GaBi, SimaPro, and the EcoInvent Database. The correction of these errors will hopefully reduce uncertainty and bias in future LCA studies.

7.4 Enabling optimization in LCA: from the ad hoc to the Structural LCA approach

- ***Based on a biodiesel well-to-wheel case study***

Applied life cycle assessment (LCA) studies often lead to comparison of rather few alternatives. We call this the "*ad hoc* LCA approach". This can seem surprising since applied LCAs normally cover countless options for variations and derived potentials for improvements in a product's life cycle. In this paper an alternative approach to the *ad hoc* method is suggested, which we call the "Structural LCA approach". The goal of this paper is to: 1) provide basic guidelines for the Structural approach, including an easy expansion of the LCA space; 2) show that the Structural LCA approach can be used for different types of optimization in LCA; and 3) improve transparency of the LCA. The Structural approach is demonstrated with an applied case study on production and use of biodiesel.

The Structural approach is based on the methodology "Design of Experiments" (DOE) (Montgomery 2005). Through a biodiesel WTW study we demonstrate a generic approach to applying explanatory variables and corresponding impact categories within the LCA methodology. Furthermore, using the Structural approach enables two different possibilities for optimization: 1) single-object optimization (SO) based on the response surface methodology (Montgomery 2005), and 2) multi-object optimization (MO) by the Hyper-volume Estimation Taboo Search (HETS) method. HETS enables MO for more than 2 or 3 objects. HETS has been developed for the current project by the Operation Research-group at Technical University of Denmark and is documented in Lundberg-Jensen (2011).

In Tables 3 and 4 below, the results for SO is presented. The explanatory variable "use of residual straws from fields" is, by far, the explanatory variable that can contribute with the highest decrease of climate change potential. For the "respiratory inorganics" impact category, the most influencing explanatory variable is found to be the use of different alcohol types, such as bioethanol or petrochemical methanol. Based on MO, we found the Pareto front based on five different PWs that are non-dominated solutions out of 66 different PWs/solutions. Given that there is a fixed amount of resources available for the LCA practitioner, it becomes a prioritizing problem whether to apply the Structural LCA approach or not. If the DM only has the power to change a single explanatory variable, it might not be beneficial to apply the Structural LCA approach. However, if the DM has the power to change multiple explanatory variables, then the Structural LCA approach seems beneficial for quantifying and comparing the potentials for environmental improvement between the different explanatory variables in an LCA system.

Table 3. Optimization potentials of climate change potential based on effect estimates and sum of squares. Abbreviations: Fert = fertilizer; Straw = use of residual straw from field; Trans = transesterification process; Alc = alcohol; and Transp = transport.

	Effect estimate/ [kg CO_2-eq.]	**Sum of squares**	**Percent (%) contribution**
***Intercept* (µ)**	79.54		
Fert (+)	13.20	2,788	3.0
Straw (+)	-73.55	86,554	92.3
Trans (enz)	2.28	83	0.1
Alc (PCMe)	11.13	1,982	2.1
Electricity (PL)	1.66	44	0.0
Transp (+)	12.06	2,328	2.5

Table 4. Optimization potentials of respiratory inorganics based on effect estimates and sum of squares. Abbreviations: Fert = fertilizer; Straw = use of residual straw from field; Trans = transesterification process; Alc = alcohol; and Transp = transport.

	Effect estimate/ [kg 2.5PM-eq.]	**Sum of squares**	**Percent (%) contribution**
***Intercept* (µ)**	0.0711844		
Fert (+)	0.0070750	0.0008009	7.0
Straw (+)	-0.0048688	0.0003793	3.3
Trans (enz)	-0.0002000	0.0000006	0.0
Alc (PCMe)	-0.0230313	0.0084870	74.6
Electricity (PL)	0.0043188	0.0002984	2.6
Transp (+)	0.0093750	0.0014062	12.4

The illustration and implementation of the Structural LCA approach and the derived use of SO and MO has been successfully achieved and demonstrated in the present paper. In addition, the structural LCA approach can lead to more transparent LCAs since the explanatory variables used to model the LCAs are explicitly presented through the Structural LCA approach. The suggested Structural approach is a new approach to LCA and it seems to be a promising means of searching or screening product systems for environmental optimization potentials. In the presented case, the design has been a rather simple full factorial design. More complicated problems or designs, such as fractional designs, nested designs, split plot designs, and/or unbalanced data etc. could be investigated further in the context of LCA.

The relation to the statistical value chain

This paper takes the LCA of biodiesel from a WTW perspective which was hooked on a "step 4" in the statistical value chain in the previous paper "Potentials for optimized production of biodiesel in a well-to-wheel study" and brings the biodiesel WTW study to a "step 7" level. However, only a few (65) alternatives are compared with the baseline study "PWA1" in contrast to what is theoretically possible in a normal LCA used for decision support. Potentially thousands of different PWs should be possible in applied LCA studies due to the vast amount of combination possibilities. These potential different PWs, I would suggest, comes from alternations of a retrospective LCA, whenever it is possible. That is, the AN, DM and experts suggest possible PWs that potentially could be developed – few alternations of different explanatory variables can quickly turn into thousands of different options (PWs). The baseline in this study has been forecasted with the "*Naïve forecast method*". This also means that the baseline is sensitive to any changes, both exogenous as well as endogenous. For this reason, it seems reasonable to assume the same delimitation of the Repetitively dimension, namely $P_{(t+1)}–P_{(0)} \rightarrow 0$.

Further discussion

It must be considered that optimization based on bias and uncertainty data can lead to the risk of incorrect decision support. In the context of the errors and bias seen in the paper "Does it matter which LCA tool you choose? - comparative assessment of SimaPro and GaBi on a biodiesel case study" it might be worth eliminating such errors and bias before stepping up to a "step 7" in the statistical value chain.

Value-adding

Given that data are suitable and unbiased, then the Structural LCA approach, which has been imported from the Design of Experiments methodology, seems to be value adding to the LCA field.

8 Outlook and concluding remarks

As an outlook the following four topics are presented:

1. The PhD project summarized into one equation
2. How to keep track of all the changes in a long running LCA project used for decision support
3. Market forces in LCAs used for decision support
4. Do numbers used for decision support have a "supporting" capacity (limit)?

These topics have not explicitly been presented elsewhere in this dissertation and I think they can either be considered "take-home messages" from this PhD project or they can be used as inspiration for further research that can be value-adding to the general LCA field.

8.1 The PhD project summarized into one equation

One of the main findings in this PhD project is the relation between three different explanatory variables (defined below) and the response variable "uncertainty". This relation is expressed in Equation 1 below:

Equation 1

$$f(A, B, C) = U$$

Where $$U > \alpha \geq U$$

"A" are the resources available for the AN; "B" is the size of LCA space investigated; "C" is the capability of the AN; "U" is the uncertainty level; "α" = *accepted* uncertainty level set by the DM.

The explanatory variables "A" and "B" have been elaborated to a great extent throughout this PhD thesis ("B" is outlined in the pedigree matrix). "C" has to a smaller extent been elaborated in this PhD thesis. For example, the more the AN deviate from procedures laid out in the statistical value chain the more errors, bias, and uncertainty I would expect to occur in a given LCA. In other words this explanatory variable covers the AN education level.

I will claim that there is no possible way to "overcome" or compensate this relationship by applying any algorithm or a simulation tool. The equation can be used to understand what drives uncertainty in LCAs used for decision support.

I assume that the understanding of uncertainty expressed in Equation 1 belongs to the rational school of management. As discussed in the subsection "Transparency: Confronting *obscurity* in LCA used for decision support"[7], obscurity can also be a source of uncertainty but this understanding of uncertainty I assume belongs to the Anarchistic school of management.

8.2 How to keep track of all the changes in a long running LCA project used for decision support?

During the three years that that PhD project has lasted, I have presented LCA results to the DMs in the "Project Platform"[8] several times. I have used a great part of my time at these presentations to explain and discuss different LCA related assumptions with the DMs who are not familiar with the LCA methodology rather than using time to discuss how my findings could lead the project in a more sustainable direction. Many times I had to start with "the beginning" when presenting the latest LCA results. This problem I would assume could partly have been avoided if throughout the project period I had used a consistent framework for keeping track of changes from presentation to presentation. Since most of the stakeholders in the Project Platform are scientists I would also assume that they are familiar with statistics and "effect models" as presented in the paper "Summary - Enabling optimization in LCA - from the *ad hoc* to the Structural LCA approach in LCA". If from the start of the project period I had used a very simple effect model (say with two or three explanatory variables) and from presentation to presentation had developed this model I would assume that: 1) the different Project Platform stakeholders would have experienced the presentations as being more consistent and 2) it would have been much easier for the different stakeholders to keep track of changes in the LCA model from presentation to presentation. The key in this approach is that every *change* in the response variables strictly explained by a *change* in an explanatory variable is *explicitly* expressed. In a longer lasting and similar LCA project in the future I would consider using such an approach, i.e. the Structural LCA approach, and continuing to develop the model throughout the project period.

[7] Further discussion. Transparency: Confronting *obscurity* in LCA used for decision support" in the chapter "Summary - Confronting uncertainty in LCA used for decision support
[8] see Preface to recapture the DMs in the Project Platform

8.3 Market effects in LCA used for decision support

Changing a product, or putting a new product on the market, can potentially change the market structure. Not including market effects in the LCA does not mean that such market effects do not happen. If a company owner (or any DM) makes endogenous environmental process improvement (such as lowering the energy consumption in the production process) and in addition lowers the price of the product then this could (*ceteris paribus*) result in an overall *increased* market environmental impact due to an increased trade of the product. The *overall* environmental impact from the market is obviously the main interest of the society. However, whether the company owner should be held responsible for the overall market impact and, to some extent, exogenously[9] given environmental impacts in the market or not is an "*ought*-issue". A problem that can arise with ascribing environmental impact to a producer in this way is that it can jeopardize any motivation for the company owner to make endogenous environmental improvements in the production. In general, I think, that some problems arise regarding the market effects:

1. The company owner is made responsible for changes in the "overall environmental impact of the market" where much of this environmental impact can originate from exogenously given changes in the market.

2. The documentation of the causality between the company owner's product and the change in the overall market impact. In other words that the overall changes are due to this product and not something else happening in the market.

3. Given that the market experiences a high level of fluctuations such as one day the overall market's environmental impact is positive and another day it is negative, then how does the DM/company owner respond to this in the case that he is made responsible for the overall market environmental impact.

4. If the LCA can be affected by the market conditions and exogenous changes then the company owner (and the LCA) may become sensitive towards other players in the market that act in a strategic way to influence the LCA of the company.

[9] Exogenous forces are forces (or variables/changes) that the DM cannot (or at least not easily) influence - they are imposed from "the outside". Endogenous changes are influenced by the DM's choice among the existing alternatives.

One way to deal with such a problem could be: A) let the company owner make the environmental improvements of the product, and B) let the regulatory authorities handle the market's overall environmental impact. I think it is relevant to consider these issues when further developing the LCA field used for decision support. In Mulalic (2011), rebound effects of the improvement of truck engines efficiency are investigated with the conclusion that the *overall* environmental impact of the market can be worse when truck engines efficiency are improved.

8.4 Do numbers used for decision support have a "supporting" capacity (limit)?

In physics a battery has a capacity, defined as the amount of electric charge that the battery can store. Hui (2006) uses the concept "carrying capacity" as the ability of an environment to sustain populations. Different fluids have different heat capacities. In communication engineering channel capacity is the upper bound of information that can be transmitted over a communications channel. In the same way I will here, as a final outlook for further consideration, ask the question:

Do numbers used for decision support have a "supporting" capacity (limit)?

If different physical items as exemplified above have capacity limits, why should numbers used for decision support not equally have supporting capacity limits? For example, Royal Society (1992) discusses how communication (and numbers) from a scientific community are *in general* perceived by many DMs and the general public as being numbers that are credible, with low bias and low uncertainty. This would indicate that, yes, numbers from a scientific community do have a supporting capacity limit which is related to the uncertainty inherent in the numbers. This could perhaps be a topic for further research.

8.5 Expanding the idea of Hume's "is-ought" problem

I would here like to expand the idea of Hume's "*is-ought*" problem. In a strictly physical sense the state of the world can be described by Equation 2 as formulated below. How the world is at present I would consider as an "is-issue". How the state of the world "should be" in the future is an "ought-issue". Equation 3 is related to this "ought-issue". An important distinguishing here is that both equation 2 and 3, at any point in time which is "present" will be completely determined. Changing the physical and present state of the world can only be done by people alive[10] and *ought* to be done, I would think, in accordance with their expectations of what will maximize W over time.

In the following vector model $E = (E_t)_{t\in\mathbb{R}}$ (Equation 2) it is assumed that the Solar system is an isolated object consisting of N elements. Each element is undividable small at all times. Let E describe their positions with the origo in the center of the earth at time t:

Equation 2:

$$E = \begin{bmatrix} e_{(t,1,x)} & e_{(t,1,y)} & e_{(t,1,z)} \\ \vdots & \vdots & \vdots \\ e_{(t,i,x)} & e_{(t,i,y)} & e_{(t,i,z)} \\ \vdots & \vdots & \vdots \\ e_{(t,N,x)} & e_{(t,N,y)} & e_{(t,N,z)} \end{bmatrix}$$

The subscripts are; at time t particle i has the position of the vector coordinates (x,y,z). Based on this vector function a "Value function" can be constructed (developed from the welfare theorem outlined in Møller (1996)) for each person in the world at all times:

Equation 3:

$$W = \sum_{t=0}^{T} \sum_{h}^{n} f_h(E_{t,h})$$

W gives the value of the state of the world for all humans, h sums over all people in the world at all times, and f is the preference function for each person.

This is the last "hook" for how, I think, the overall goal of environmental engineering and sustainability thinking could be perceived. Based on this idea a further research topic could be an investigation of any types of hazards which could jeopardize the goal of maximizing W. Such hazards could for example be: nuclear power accidents, emission of green house gasses, super volcano eruptions, pandemics, sun blasts etc., as discussed by WEF (2010) or Faber (2011).

[10] And/or exogenous given forces.

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10 List of conference proceeding, seminar, and appendix of full length papers

Peer reviewed journal papers as first author:

A. Confronting uncertainty in LCA used for decision support - Developing a taxonomy for LCA Studies (2012)
B. Potentials for optimized production of biodiesel in a well-to-wheel study (2012)
C. Does it matter which LCA tool you choose? - Comparative assessment of SimaPro and GaBi on a biodiesel case study (2012)
D. Enabling optimization in LCA - from the ad hoc to the Structural LCA approach in LCA - based on a biodiesel well-to-wheel case study (2012)

Peer reviewed journal paper not as first author:

E. Assessing the greenhouse gas emissions from poultry fat biodiesel (2012)

Popular journal paper (not peer reviewed), conference proceeding and seminar:

F. Sustainable biodiesel based on enzymes [Bæredygtig biodiesel med enzyme] (2009). Only minor contribution to the paper. No co-author agreement has been found necessary to submit.
G. Ivan T. Herrmann. Environmental Sustainability Analysis of Biodiesel Production: A Comparative Analysis of Different Production Schemes. Platform presentation at The American Oil Chemists' Society Conference. May 5, 2009. Orlando, FL, USA.
H. Ivan T. Herrmann. Sustainable climate solutions. Workshop for high school teachers. September 29, 2009. Søhuset SCION, Hørsholm, Denmark.

Appendix A: Confronting uncertainty in LCA used for decision support - Developing a taxonomy for LCA Studies

Authors: Ivan T. Herrmann, Michael Z. Hauschild, Michael D. Sohn, and Thomas E. McKone

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Title: Confronting Uncertainty in LCA Used for Decision Support

Subtitle: - Developing a Taxonomy for LCA Studies

Ivan T. Herrmann*, Michael Z. Hauschild, Michael D. Sohn, and Thomas E. McKone

Address to correspondence to:
*Corresponding author: ivan.t.h.business@gmail.com

Section of Quantitative Sustainability Assessment, Department of Management Engineering, Technical University of Denmark, Room 130, Building 426, Produktionstorvet, DK-2800, Kgs. Lyngby, Denmark

1 Summary

The goal of this article is to present a taxonomy of terms used to explain and classify the uncertainty one faces in Life Cycle Assessments (LCA). LCA offers a quantitative approach to assessing environmental impacts from products, technologies and services. LCAs are conducted by LCA practitioners or analysts to help decision makers map the tradespace between various competing attributes, which may include protection of near- or far-field environmental quality, maximizing economic benefits, and improving production timelines. At present, some decision makers may have reservations against LCA as a reliable decision support tool due to the perceived crude manner in which uncertainty has been dealt with in LCAs in the past, and the large uncertainties that are sometimes reported in the LCA literature. Many researchers are developing algorithms and processes to better quantify and compute uncertainty in end results. In this article, we provide a higher level explanation of uncertainty in different types of LCAs based on the taxonomy and the Law of Large Numbers. It is the hope that the taxonomy will provide life cycle analysts, decision makers, and other stakeholders with a common language to describe the certainty, and intrinsic obscurity, of LCAs and will therefore improve the planning of an LCA to be performed and the effective interpretation and application of the LCA results.

Keywords: LCA space, variability, transparency, obscurity, Law of Large Numbers.

2 Introduction

Life Cycle Assessment (LCA) offers a quantitative approach to assess environmental impacts from products, technologies and services (Wenzel et al. 1997; Finnveden et al. 2009; European Commission 2010). LCA's are conducted by LCA practitioners or analysts (AN) to support decision makers (DM) in making sound choices, amongst many competing attributes, for a given decision support context.

At present LCA is still not fully endorsed or used by some DM's for decision support due to the perceived crude manner in which uncertainty has been dealt with in LCAs in the past (Bras-Klapwijk 1999). Bjorklund (2002) asks for an LCA framework, which is not too complex to apply, and can address the problem of reliability in an LCA. Malça and Freire (2010) and McKone et al. (2011) point out that uncertainty is (still) a major challenge for LCAs. The present article addresses these problems by:

A) Developing a taxonomy that we think can be useful to classify different types of LCA's used for decision support.
B) Showing how this classification system can be used to understand, rank, and hence confront uncertainty in LCA used for decision support.

We believe that one reason why some DM's may not fully endorse LCA practices is because they consider the uncertainty of the results to be too high or because they believe that it has been underestimated or even ignored as indicated by Weidema (2009). As methods to quantify uncertainty are being developed, a key step is improving how uncertainty and variability is communicated in an LCA; a suite of terms that serves as a common language to discuss LCA results could expand the interpretation of LCAs. Rooted in the simple probability principle expressed in the Law of Large Numbers (LLN) a consistent, though not comprehensive, list of terms is developed. Throughout, we give concrete examples of the taxonomy put into practice.

The LLN is here interpreted as: "*when keeping the sample size (n) constant then the estimated average based on the sample will be a less accurate estimate of the true population average as the population size (N) increases*". For more information about the LLN see Loève (1963) or Pitman (1993). Furthermore, we assume that *N* can be interpreted as the *space* which we are making LCA statements about. An LCA statement is the answer to an LCA question (or inquiry). As a theoretical example consider two different LCA questions concerning biofuels:

Q1. "What is the environmental impact of producing 10 tons of bioethanol in a specific company in Brazil today based on sugar cane?"

Q2. "What is the environmental impact from the total Brazilian production of bioethanol of today?"

The two questions differ significantly in terms of the size of the space under investigation. Q1 focuses on one specific company in Brazil while Q2 is looking at all companies in Brazil that produce bioethanol (>100). The LCA space of Q2 is larger than for Q1. If the DM wants these questions to be answered with the same level of certainty then the AN needs significantly more resources[i] for data gathering for Q2 compared to Q1. On the other hand if the resources for data gathering are fixed then the uncertainty of the answer to Q2 will increase compared to Q1. The key assumption of this article is that there are two main variables that fundamentally determine the uncertainty of an LCA. These two variables are:

i. The resources available for the AN
ii. The size of the LCA space about which inquiries are made

It is assumed that both variables (i and ii) can be ranked on a continuum going from small to large. These two variables are clearly very influential on the final uncertainty of the LCA statement. As the LLN suggests – there will always be a trade-off between how all-embracing the assessment is and how uncertain the assessment is. In addition to these two aspects it is also possible that DMs have different *accepted* uncertainty levels. For example, instead of accepting a +/- 10 % uncertainty range a DM can accept an uncertainty range of +/- 110 %. The accepted uncertainty level is kept constant throughout most of this article and hence it is possible for the uncertainty of the LCA statement to be either: lower than; equal to; or higher than the DM's accepted uncertainty level.

In statistics, uncertainty is considered a function of the sampling procedure and the sample size (n) compared to the population size (*N*) (Cochran 1977). To avoid biases in results based on data collection, a suitable randomization in the sampling procedure, as described in theory of sampling, is a strong prerequisite (Gy 1998; Petersen, Minkkinen, and Esbensen 2005).

Several authors (Ross et al. 2002; Huijbregts et al. 2003; Ciroth et al. 2004; Heijungs and Huijbregts 2004; Heijungs and Frischknecht 2005; Lloyd and Ries 2007) have proposed different approaches for identifying and quantifying uncertainty in LCA. The general approach suggested in these articles is summarized in the three-step procedure below, which is basically a limited exercise in variance propagation:

- Collect data, (normally from the literature and often resulting in single point estimates) Estimate variation or uncertainty range for individual data (expert guesses or estimates, for example "+/-10 %" as suggested in Huijbregts et al. (2001) or using the pedigree reliability matrix developed in Weidema and Wesnæs (1996).
- Apply Monte Carlo or similar simulation tools to propagate variation ranges and model uncertainty.

Such a procedure for uncertainty assessment cannot be considered in agreement with theory of sampling, and it has the risk being biased or underestimating the true uncertainty level, leading to an incorrect decision support. Only one article was found (Huijbregts 1998) observing that it may not be possible to actually quantify or reduce (model) uncertainty in LCA when it arises from lack of information.

Throughout the article it is assumed that there will be a fixed amount of resources for the AN and that the uncertainty of the LCA statement will vary with the size of the LCA space about which inquiries are made. Therefore the focus is on how the LCA question can be scaled and for this discussion the developed taxonomy is instrumental.

3 Taxonomy for Classification of LCA Studies

In the following section a taxonomy for classification and description of uncertainty in LCA used for decision support is presented and explained. The development of the proposed taxonomy has been inspired by studying a range of LCAs, applied as well as more theoretical ones, in particular: Huijbregts (1998); Wenzel (1998); Hertwich et al. (2000); Huijbregts et al. (2001); Weidema (2001); Weidema (2003); Ciroth et al. (2004); Ekvall and Weidema 2004; Ciroth (2006); Lloyd and Ries (2007); Harding et al. (2008); Searchinger et al. (2008); Sander and Murthy (2010); Schmidt (2010); McKone et al. (2011); Sanz Requena et al. (2011); Varanda et al. (2011). As such, the present taxonomy is deduced from this literature with further inspiration in both the management and the economic literature. Two LCA case studies Schmidt (2010) and Sander and Murthy (2010) are discussed and used for an exemplification in section "Demonstration of the Use of the Pedigree Matrix". In the "Concluding Remarks" section the taxonomy and its use for uncertainty classification are discussed from a management and decision support perspective.

3.1 Dimensions of the Taxonomy

The taxonomy operates with six dimensions each varying between two extremes. The six dimensions are summarized in table 1.

Table 1 Dimensions used to classify LCA studies.

Tangibility **Tangible (T) vs. Intangible (I)**	Tangible things can be measured and touched in the corporeal world. In contrast intangible things can be ideas or concepts. Only hypothesis and indirect evidence can be made about intangible things.
Time **Retrospective (R) vs. Prospective (P)**	Retrospective studies deal with what happened in the past while prospective studies involve estimation of future events.
Repetitivity **Single-period (S) vs. Multi-period (M)**	Single-period is for example the CO_2 emission from a given factory in 2008. For multi-period it is for more than one year, say 2007, 2008, and 2009.
Change **Baseline (B) vs. Change (C)**	Baseline is business as usual while a change is considered anything different from the baseline.
Scale **Micro (i) vs. Macro (a)**	A relative size scale. Micro is small compared to macro, but the absolute scale depends on what is relevant for the studied function or service.
Value **Physical (Y) vs. Value (V)**	Physical refers to the location and quantity of matter and energy in time and space. Value refers to the value placed on that same physical entity by one or more DM's.

The dimensions are constructed as a "point-of-departure" starting from the *left* extreme. As an example, take the dimension Repetitivity going from single-period to multi-period. Evidently the multi-period type of study consists of more than one single-period, hence this dimension must always start with a single-period. Moving from left to right, that is from a single-period study to a multi-period study means increasing the LCA space. Assuming that most product systems change over time and with a fixed amount of resources for the AN, the uncertainty will increase as the LCA used for decision support are assumed to represent more time-periods. The six dimensions are elaborated in the section "The six Dimensions" below.

3.2 Ranking the LCA Studies According to Inherent Uncertainty

Figure 1 combines the six dimensions into a pedigree matrix for classification of LCA studies. For each dimension the two extremes are shown in the matrix resulting in 64 possible classifications. The pedigree matrix has been ordered in a way where all the left extremes for each dimension in table 1 are placed *before* the right extremes, starting from the upper left corner. The order between the six dimensions has no relevance for the interpretation of the pedigree matrix. The classifications are relevant for estimating the level of inherent uncertainty that the study is prone to according to the LLN and the degree of inference involved in the study. The classification index is formed from the abbreviation code for each extreme in the six dimensions. For example if the LCA inquiry calls for an LCA involving tangible, multi-period, micro, retrospective, changes, and physical – then the index code for this LCA inquiry is: TMi-RCY, where the dash only serves to ease the reading of the code. In general, an index number involving the high extremes of the dimensions will lead to a higher inherent uncertainty. For example going from micro (i) to macro (a), going from single-period (S) to multi-period (M), going from baseline (B) to change (C), and so forth will increase the inherent uncertainty, when keeping the resources constant for the AN. The upper left corner starting with the TSi-RBY LCA gives the lowest possible LCA space, while the lower right corner ending with the IMa-PCV LCA gives the largest possible LCA space. This means that moving an LCA study (by changing the scope definition) from the upper left corner to the lower right corner of the matrix will increase the inherent uncertainty of the LCA used for decision support when keeping the resources constant for the AN, as indicated by the arrow.

			Tangible (T)				**(Tangible +) Intangible (I)**			
			Single-period (S)		**Multi-period (M)**		**Single-period (S)**		**Multi-period (M)**	
			Micro (i)	**Macro (a)**	**Micro (i)**	**Macro (a)**	**Micro (i)**	**Macro (a)**	**Micro (i)**	**Macro (a)**
Retrospective (R)	**Baseline (B)**	**Physical (Y)**	TSi-RBY	TSa-RBY	TMi-RBY	TMa-RBY	ISi-RBY	ISa-RBY	IMi-RBY	IMa-RBY
		Value (V)	TSi-RBV	TSa-RBV	TMi-RBV	TMa-RBV	ISi-RBV	ISa-RBV	IMi-RBV	IMa-RBV
	Change (C)	**Physical (Y)**	TSi-RCY	TSa-RCY	TMi-RCY	TMa-RCY	ISi-RCY	ISa-RCY	IMi-RCY	IMa-RCY
		Value (V)	TSi-RCV	TSa-RCV	TMi-RCV	TMa-RCV	ISi-RCV	ISa-RCV	IMi-RCV	IMa-RCV
Prospective (P)	**Baseline (B)**	**Physical (Y)**	TSi-PBY	TSa-PBY	TMi-PBY	TMa-PBY	ISi-PBY	ISa-PBY	IMi-PBY	IMa-PBY
		Value (V)	TSi-PBV	TSa-PBV	TMi-PBV	TMa-PBV	ISi-PBV	ISa-PBV	IMi-PBV	IMa-PBV
	Change (C)	**Physical (Y)**	TSi-PCY	TSa-PCY	TMi-PCY	TMa-PCY	ISi-PCY	ISa-PCY	IMi-PCY	IMa-PCY
		Value (V)	TSi-PCV	TSa-PCV	TMi-PCV	TMa-PCV	ISi-PCV	ISa-PCV	IMi-PCV	IMa-PCV

Figure 1 Pedigree matrix for LCA studies showing the 64 different types of LCA's with corresponding inherent uncertainty, when keeping the resources constant for the AN. Moving from the upper left corner to the lower right corner the expected uncertainty will increase. The index system can be used to describe which type of LCA question will hold the most uncertainty. The index system is formed from the abbreviation code for each dimension. For example if the LCA question involves tangible, multi-period, micro, retrospective, changes, and physical – then the index code for this LCA problem is: TMi-RCY.

4 The Six Dimensions

To ease the understanding of three of the dimensions a short theoretical biodiesel case is introduced below. The three dimensions are: “retrospective versus prospective”, “single-period versus multi-period”, and “baseline versus change”.

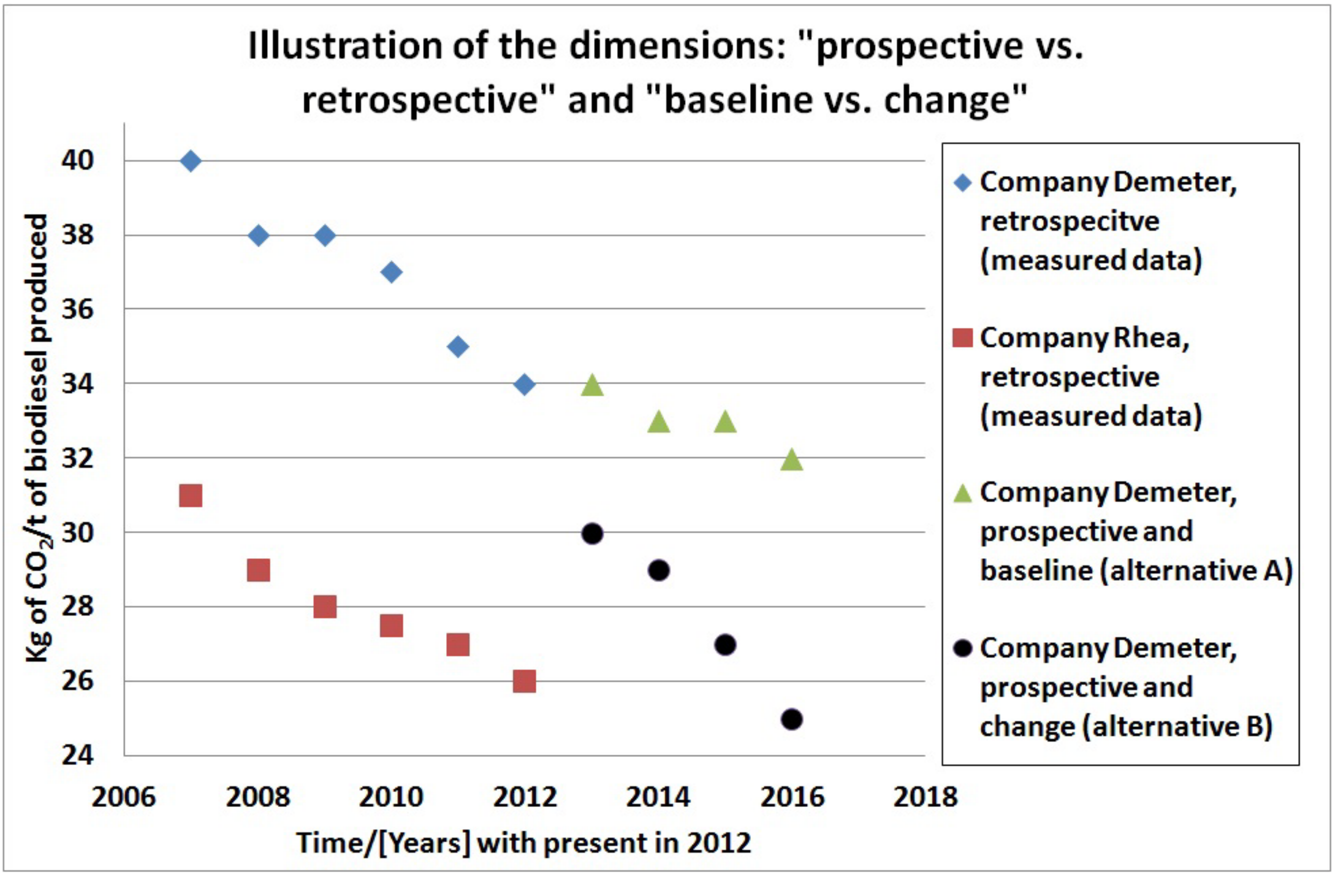

Figure 2 Illustration of the three dimensions Time perspective (prospective vs. retrospective), Periodicity (single-period vs. multi-period) and Change (baseline vs. change), where the baseline is understood as business as usual (triangle points). The case is a fictive business case of biodiesel production with two different types of transesterification processes.

Consider two companies: “Demeter” and “Rhea” both producing biodiesel. The case is illustrated in figure 2. First consider the time period from 2007 to 2012 (multi-period or 6 single-periods). The company Demeter uses a conventional chemical transesterification process for converting biomass feedstock into biodiesel while the company Rhea uses an enzymatic transesterification process. In

2011 Demeter gets an offer from an enzyme producing company to buy enzymes that can do the transesterification process (alternative B) at the same monetary price as if they continued with the conventional transesterification process (alternative A – the baseline based on business as usual). Demeter starts looking for arguments that can support their decision whether to proceed with business as usual or change to the enzymatic transesterification process. The enzyme-producing company has already sold the same enzymes to the company Rhea for a period of years. Both companies Demeter and Rhea have for some years monitored their environmental performance in terms of CO_2 emission per produced t of biodiesel. Based on these retrospective and measured data it turns out that environmentally the CO_2 emission of the enzymatic process is clearly favorable compared to the conventional transesterification process. These data supports Demeter's decision to change their production method. It is then *forecasted* (4 single-periods – 2013, 2014, 2015, and 2016) how much this *change* in production method (going from alternative A to B) will result in an improved environmental performance which can be calculated as the difference between the prospective baseline (alternative A) and the prospective alternative (alternative B).

In the following subsections a presentation is given to the theoretical background for each of the six dimensions, and we try to demonstrate the relevance of the taxonomy to LCA.

4.1 Tangibility

The theoretical background for the Tangibility dimension is taken from the service management literature. The classification "tangible" covers things that can be touched and seen. They are real and exist in the corporeal world (Fitzsimmons and Fitzsimmons 2006). Having a ton of biodiesel at hand is tangible and can be measured directly. The classification "intangible" covers things with incorporeal properties, that is ideas and concepts that cannot be seen or touched. It is possible to measure a ton of petrochemical diesel or biodiesel but, as an example of intangibility, it is hard to measure a person's feeling toward the incineration of the biodiesel (Grönroos 2000).

In LCA *substitution* can be used to solve LCA problems with multifunctional processes with more than one output (and/or input) assuming that product A will replace product B in the market (Weidema 2003; Ekvall and Weidema 2004). This statement involves two assumptions: 1) a certain amount of product B was not (or will not be) produced, and 2) that the "not produced" amount of product B has a (quantifiable) causality with the produced amount of product A. That something is not produced implies that it does not exist in the corporal world hence we regard this as being intangible. In the section “Demonstration of the Use of the Pedigree Matrix” the LCA study of Schmidt (2010) is analyzed for intangible effects and it is found that in this case it can lead to some uncertainty and derived potential flaw for decision support. To derive *correct* and non-biased substitution and market effects from different data sets can be rather resource-intensive (Mathiesen et al. 2009; Salmon 2009; Mulalic 2011). Alternative methods for solving multi-functionality problem in LCA exist (Wenzel et al. 1997; Finnveden et al. 2009). These methods can be less resource demanding. We believe that the most appropriate solution depends on the decision support context. The decision support context is discussed in the section “Concluding Remarks”.

4.2 Time Perspective (Retrospective or Prospective)

The influence of this dimension for the inherent uncertainty of the LCA lies in the fact that we can know about the past with somewhat close to certainty if proper data collection has been done for the considered product systems. For forecasting or prospective analysis we must rely on informed assumptions, qualified guesses or expectations about what will happen in the future, as illustrated with the above biodiesel case (for alternative A and B). As a result the potential outcome space[ii] will inevitably increase and the LCA results will become more uncertain compared to a strictly retrospective analysis. No prospective LCA can be better than the retrospective data that form the basis for the forecasting. In the LCA literature retrospective and prospective assessments are discussed in for example Weidema (2001) and Weidema (2003).

4.3 Repetitive Studies (Single-period versus Multi-period)

The dynamic nature of most product systems makes this dimension important for LCA. For illustration consider the above theoretical biodiesel case, where each time-period corresponds to one year. This is a case of a multi-period LCA (10 periods). The influence on uncertainty from this dimension comes from the fact that multi-period studies require more work (even if many parts are similar between the individual periods). Each time a period is added, then (in general) the result will be more uncertain if the resource for the AN is kept constant.

In the LCA literature examples of single-period studies are Sander and Murthy (2010) and Hansen (2007) while multi-period studies are found in Shui and Harriss (2006); Herrmann and Hauschild (2009); Schmidt (2010). The theoretical background for the single-period versus multi-period dimension is inspired by the book “Forecasting – methods and applications” (Makridakis 1998).

4.4 Change

The theoretical foundation for this dimension can be found in the optimization literature as for example Lindeneg (1998). Building on the theory that decision support is about finding the best of several alternatives then a baseline is (always) needed before judging whether other alternatives are better. This also implies that the first step must be to determine a (realistic and relevant) baseline – as illustrated in the above biodiesel case as alternative A. As a good definition for a baseline study we propose:

"*describe exactly what (you think) will happen if the change under consideration was <u>not</u> introduced*"

This also implies that the "next step" is to describe other alternatives. In the biodiesel case above alternative A is the baseline and alternative B is the second alternative. We assume, with a fixed amount of resources for the AN, the more uncertain the result will be with an increased number of alternatives. Both exogenous and endogenous forces[iii] on the investigated production system are relevant to consider since both types of forces can profoundly impact the considered baseline, as well as the considered alternatives, and hence if not considered this can lead to flawed decision support (Knudsen 1997; Johnson et al. 2005). In the LCA literature, such as European Commission (2010), the application "environmental product declaration, EPD" can be considered similar to the isolated baseline since it only describes a product as it is (or will be) and not necessarily compares it to an alternative.

4.5 Scale (Micro versus Macro)

The scale influences the uncertainty of the LCA results in two different ways. The first way is that; if the size of the LCA space that is investigated is denoted N then it can be seen from the LLN that as N grows, which is the case when going from micro to macro, then the uncertainty will also increase when the resources for the AN is kept constant. The case from the introduction section with Q1 and Q2 is an LCA example of going from micro to macro level.

The micro and macro levels have to be interpreted as relative terms. It is necessary to compare a given LCA to something else before it can be judged as being at a micro or macro level, although, larger projects on regional and country level such as infrastructure projects might be regarded as macro scale studies while smaller projects such as individual product assessments might be regarded as micro scale.

The second point is inspired in the economic literature such as Møller (1996) and Lindeneg (1998) who operate with projects inducing marginal changes or structural changes. The nature of the induced change relates directly to the scale. According to Møller (1996), micro projects will not change the price vector in the economy, while structural projects will. This also implies that if an LCA is regarded as being on a micro level, substitution effects equal *zero*, which means that no substitution necessarily will take place. As with the Q1 and Q2 from the introduction it can (in many cases) be possible to scale the LCA question by the amount of units that are desired to include in the LCA. If the LCA question is scaled to a level where structural changes are expected to begin to occur then a simple scaling is inadequate and appropriate alternative methods should be applied as suggested in Møller (1996) and Lindeneg (1998).

4.6 Value

Physical refers to the location and quantity of matter and energy in time and space. Value refers to the value placed on that same physical entity by one or more DM's. As an example, consider the biodiesel case above where the CO_2 emission from production of biodiesel from Demeter in 2011 was 35 kg CO_2/t. These quantities (CO_2 and biodiesel) refer strictly to physical matter and energy in time and space. How different people valuate these quantities is fundamentally another question and valuation of such quantities (especially quantities characterized as being externalities) are difficult and time consuming according to for example Hanley et al. (2007). If the DM only has one criterion, as illustrated in figure 2 (CO_2 emission), *and it can be assumed that less is (always) better than more* in an environmental context, then it might be unnecessary (additional step) to make valuation of the physical quantities. Theories for *multi-objective* decision making are discussed in Møller (1996) and Lindeneg (1998) including a broader perspective of challenges that arise with multi-objective optimization. Specifically for LCAs, multi-objective optimization has been applied in studies by: Azapagic (1999); Azapagic and Clift (1999a); Azapagic and Clift 1999b); Herrmann et al. (2012).

5 Demonstration of the Use of the Pedigree Matrix

Sander and Murthy (2010) and Schmidt (2010) present two LCA studies used for decision support. We use these LCA studies for the evincing of the selected taxonomy and the inherent uncertainty in different types of LCAs according to the pedigree matrix presented in figure 1.

In the article “Comparative life cycle assessment of rapeseed oil and palm oil” Schmidt (2010) makes a consequential LCA (CLCA) and an attributional LCA (ACLA) where rapeseed oil and palm oil is compared. Five different scenarios are presented. Three scenarios are using a CLCA approach and two scenarios are using an ACLA approach. In terms of CO_2-eq and increased rape seed oil production it is found that 17.1 ton CO_2-eq is emitted per ton of increased demand of rape seed oil using a CLCA approach. Using an ALCA approach the same number is found to be 2.22 ton CO_2-eq. These numbers are respectively maximum and minimum for the five scenarios.

It is stated that the above findings are valid for a time horizon of 5-10 years starting in 2005. Hence the study is prospective and multi-period, it includes intangible effects, and it has a change perspective, at least for the CLCA approach (even that the baseline(s) is/are not entirely clear). Presumably it is a macro study. It is clearly not a “value” study. This is then an IMa-PCY LCA study, which is one of the more complicated LCA studies according to the pedigree matrix and some inherent uncertainty should be expected for this study.

The tangible facts for production of rapeseed and spring barley from Statistics Denmark (dst.dk 2011) are presented in table 2. These tangible and retrospective facts are evaluated against Schmidt (2010) intangible effects and prospective findings.

Table 2 Tangible and retrospective data from Statistics Denmark (dst.dk 2011) for production of rapeseed and spring barley for the years 2005-2009. It can be observed from these data that from 2005 to 2009 the area for rapeseed production was increased with 51.4*10^3 ha while the area for spring barley was decreased with 116.5*10^3 ha.

Tangible and retrospective data from Statistics Denmark. Production of Spring Barley and Rapeseed (2005-2009)							**Evaluation**	
Crop	**Metrics**	**Year**						
		2005	**2006**	**2007**	**2008**	**2009**	**Absolute difference (2005-2009)**	**Actual growth rate p.a. (%)**
Spring Barley	Production (mio kg)	2961.1	2374.1	2248.3	2645.5	2455.7		-5.8
	Areal (1000 ha)	565.7	520.5	461.9	588.3	449.2	-116.5	-7.7
	Average yield (hkg/ha)	52.3	45.6	48.7	45	54.7		0.3
Rapeseed	Production (mio kg)	342.2	434.7	588.6	629.2	637.4		13.8
	Areal (1000 ha)	111.7	125.4	179.2	172.1	163.1	51.4	*7.8*
	Average yield (hkg/ha)	30.6	34.7	32.8	36.6	39.1		*5.7*

The assumption in Schmidt (2010) is that 1 ha increased cultivated land for rapeseed production will lead to a decrease of 0.186 ha land cultivated for spring barley in Denmark (ratio: -0.186). From table 2 it can be observed that from 2005 to 2009 the area for rapeseed production was increased with 51.4 kha while the area for spring barley was decreased with 116.5 kha (ratio: -0.441). The "Statistics Denmark (dst.dk 2011) ratio" and "Schmidt (2010) ratio" deviate from each other with a proportion of *2.4*. The tangible and retrospective data indicate that something more than increased rapeseed production drives the decrease of land cultivated for spring barley. Potentially these other variables can drive more of the decrease of the spring barley than the increase of the rapeseed production explains.

Schmidt (2010) assumes that from 2005 and 5-10 years forward the area cultivated for rapeseed production is increased with 60% and the yield increased with 40%. The geometric means, based on 10 years, for these numbers are 4.8% p.a. and 3.4% p.a. respectively[iv]. The retrospective data for 2005-2009 shows an average increase of 7.8% p.a. and 5.7% p.a. respectively (see table 2, column "Actual growth rate p.a. %"). Based on the retrospective data and until 2009 it can be concluded that so far the trend has been different from the growth rate applied by Schmidt (2010) for the 10 years period. Whether the findings of Schmidt (2010) are acceptable or not, we believe, should be evaluated against the general decision support context and especially the DM's accepted uncertainty level.

In the article “Life cycle analysis of algae biodiesel” Sander and Murthy (2010) perform an LCA with the goal of providing baseline information for algae biodiesel process. Carbohydrates in co-products from algae biodiesel production are assumed to displace corn as a feedstock for ethanol production. Net CO_2 emissions are concluded to be −20.9 and 135.7 kg/functional unit (24 kg algae produced) for a process utilizing a filter press and centrifuge, respectively.

This study is clearly a baseline study and based on retrospective data, but intended for prospective comparisons. In addition it also includes intangible effects. Whether it is a micro or macro study is not strictly evident, but we assume that this LCA study is *not* intended to be generalized to more than the specific experiment settings; hence it can be assumed to be a micro study. Whether it is a single-period study or not is also not entirely clear. Given that the study is intended as a baseline for prospective LCAs (from 2010 and forward) it seems to be generalizing and we assume that it is a multi-period LCA. We then classify the study as being an IMi-PBY LCA study. Given that the reported (or assumed) substitution (ratio/effect) changes over time, this baseline study will deviate from the actual baseline, prospectively. On the other hand, this LCA study clearly builds on retrospective and (more or less) observed data and for that part the LCA can be classified according to the pedigree matrix, as a ISi-RBY LCA which has one of the lowest possible degrees of inherent uncertainty, given that the data collection has been done probably. We have not attempted to track data which could be used to compare and assess the uncertainty in this LCA study.

6 Concluding Remarks

We understand each cell in the pedigree matrix as representing a unique combination of switches that can be turned on or off – in other words it tells if the LCA covers intangible effects or not; if it is a macro LCA or not, and so forth. In the economic literature this corresponds to the *ceteris paribus* expression used to clarify when everything else is held constant or simply not included in a given assessment. In other words, we are *refraining* from statements of intangible effects, prospective events and so on, when these switches are "off". This is the case in the above section "Demonstration of the Use of the Pedigree Matrix" where Schmidt (2010) has the "value-switch" "off" and Sander and Murthy (2010) has both the "change-switch" and the "value-switch" off. In this way the taxonomy can support an increased transparency in the LCA decision support. The system can be used for bringing alignment between what DM's wants and what AN can deliver, given the trade-off between uncertainty and resources available for the AN. If there is no such alignment between what the DM want and what the AN delivers then this will in return lead to increased obscurity and hence uncertainty in the decision support.

Transparency is important for LCA used for decision support. The less transparent the LCA information is, the more time and resources the AN has to use to deliver the LCA results to the DM, to explain general assumptions, LCA specific assumptions, calculation methods, and so on. The developed taxonomy helps DMs, ANs, and other stakeholders with increased transparency and hereby improves the effective planning, interpretation and application of LCA used for decision support. By relating the taxonomy to the LLN we have also given DMs, ANs, and other stakeholders important insight in the relative potential uncertainty of different types of LCAs used for decision.

If an environmental study has the goal of comparing different product alternatives regarding their environmental impact potentials and the environmental study is based on different types of LCA studies found in the literature then there might be a risk of over- or underestimating one of the alternatives. As an example take the case of Demeter and Rhea, presented in the section "The Six Dimensions". If the environmental assessment of Rhea's biodiesel production includes a substitution effect[v] and the LCA study of Demeter does not include such intangible effect then this might distort the decision support if these differences are not explicitly taken into account. For this reason the developed taxonomy also seems to be value-adding.

In the introduction it was argued that the more all-embracing we aim to be with our analysis, the larger the uncertainty of the results will be. This is illustrated through the pedigree matrix presented in figure 1 and we consider this as being a fact, or "this *is* the way it really is". How to use this information, in a specific decision support context, is fundamentally another question. We believe that in principle what we *ought* to do is entirely determined by the decision support context (and especially what the DM requires). The decision support context is discussed in the following.

From the LLN it can be deduced that there are (probably) only two approaches which can be used to seriously reduce uncertainty in LCA used for decision support. That is, either to apply sufficient amount of resources for the AN or to decrease the size of the LCA space by moving towards the upper left corner in the pedigree matrix[vi]. Both approaches should lead to an alignment with the accepted uncertainty level of the DM. What the accepted uncertainty level is, is decision support context depending, simply because DM's can have different *risk*[vii] *attitudes* (Royal Society 1992; Farmer et al. 1997; Simonet and Wilde 1997). DM's can be either risk averse, risk neutral, or risk lovers (Estrin et al. 2008). That different DMs can have different risk attitudes also indicates that in a given decision support context it is difficult a priori to determine what we ought to do, that is which type of LCA should be applied. Glancing at the past can give some suggestions for different decision support contexts. Dedicated commissions supporting governmental decisions on meso- or macro scale system choices can often use considerable resources. Such commissions can work for several years and consist of a larger group of qualified experts. This type of LCA study could be a benchmark for decision support close to the lower right corner in the pedigree matrix. For the upper left corner (that is a TSi-RBY LCA) a few months with one assistant could potentially be enough, given that the DM is, what we would consider to be, risk neutral.

Different types of LCA inquiries can lead to different types of LCA strategies. For example, investigation of the potential environmental impact of establishing a biofuel production facility 5-10 years from present (LCA study A) as opposite to an LCA study where a biodiesel plant is already running (LCA study B), should lead to different strategies. With a fixed amount of resources available for the AN it is possible to prioritize how to use these resources. Using the Time dimension we can allocate all the resources either to investigate and understand a system as it is today and continue monitoring the system in more time-periods ("Deming Circle" strategy (DC-strategy)) *or* we can allocate all resources to “peer into the future” (“peering” strategy (P-strategy)). For a practical application something between these two options can be used. The DC-strategy strategy consists of four steps that are repeated continuously; plan, do, check, and act which leads to continuous benchmarking against the previous time-period. This is also a known management approach from the ISO 14000 environmental management standards. The difference between the P-strategy and the DC-strategy is illustrated in figure 3.

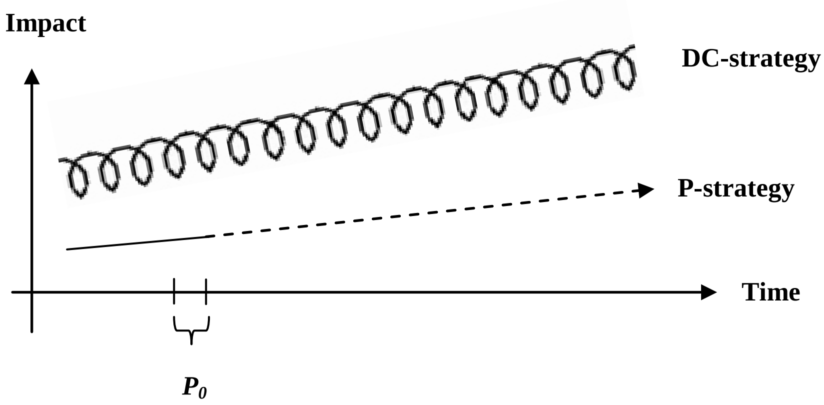

Figure 3 The DC-strategy versus the P-strategy. The dashed line indicates where the P-strategy must peer into a uncertain future. P_0 = present.

With the two LCA studies (A and B) described above and the two different LCA strategies it seems suitable to apply the P-strategy for LCA study “A” and the DC-strategy for the LCA study “B”. For the DC-strategy one of the LCA types in the upper left corner could be chosen and used repeatedly in coming time-periods, while for the P-strategy a LCA type from the lower part of the pedigree matrix should be used. It is not the intention with this framework to compare completely different projects and benchmark these against each other on an uncertainty scale. The intention is when it is possible, and we believe it is often possible, to enable that the same LCA project can be scaled according to the trade-off between the size of the LCA space and the inherent uncertainty as outlined in the pedigree matrix.

A final concluding remark is the analogous of a retrospective LCA to a company’s financial statement, which is sought to be delimited from prospective considerations of how a company *expects* (or hopes) to perform, that is prospective assessments. The financial statement is also delimited from intangible effects, for example how the company affects the market (or expects to affect the market). In Gowthorpe (2003) and Andersen et al. (2005) problems of-, how to make-, and basic assumptions of financial statement are described. Without certain standardization of financial statements (such as the US-GAAP as applied by FASB or IFRS as applied by IASB)[viii] it would have been a highly resource demanding job to analyze financial statements from different companies for comparison purpose. This analogous can serve as a benchmark for retrospective LCAs with no intangible effects such as a TSi-RBY LCA. We believe that the better described and unbiased such retrospective LCAs are the better they will serve as a starting point for prospective LCAs.

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8 About the Author

Ivan T. Herrmann is a PhD student at Section of Quantitative Sustainability Assessment, Department of Management Engineering, Technical University of Denmark in Produktionstorvet, Building 426, DK-2800, Kgs. Lyngby, Denmark. (Phone: +45 4522756975; Fax: +45 45933435)

Michael Z. Hauschild is a Professor at Section of Quantitative Sustainability Assessment, Department of Management Engineering, Technical University of Denmark in Produktionstorvet, Building 426, DK-2800, Kgs. Lyngby, Denmark.

Michael D. Sohn is a PhD in Civil and Environmental Engineering and has an M.S. degree in Engineering and Public Policy at Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA.

Thomas E. McKone is a Adjunct Professor at Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA and School of Public Health, 50 University Hall, #7360, University of California, Berkeley CA 94720.

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[i] This would also include resources that were used by other people for data gathering to make these data free and available for the AN.

[ii] For definition of outcome space we may refer to Probability theory for example (Pitman 1993).

[iii] Exogenous forces are forces/(or changes) that the DM cannot (or at least not easily) influence - they are imposed from "the outside". Endogenous changes are influenced by the DM's choice among the existing alternatives.

[iv] FV = PV(1 + i)^n -> i = (FV/PV)^(1/n) - 1. FV = future value and PV = present value. FV = 1.4 respectively 1.6, PV = 1, and n = 10. i is the yearly growth rate based on the geomantic mean.

[v] that is subtracting environmental impact from the product system

[vi] Assuming a constant efficiency level of the AN.

[vii] Uncertainty can be interpreted as the *probability* of a given event to occur, where probability, in the present article, is used interchangeable with uncertainty. The probability for a given event to occur multiplied with the quantification of the actual event is in the literature commonly treated as a *risk* (Oxford University Press 2011).

[viii] GAAP: Generally Accepted Accounting Principles - FASB: U.S Financial Accounting standards Board; IFRS: International Financial Reporting Standards – IASB: International Accounting Standards Board

Appendix B: Potentials for optimized production of biodiesel in a well-to-wheel study

Authors: Ivan T. Herrmann, Andreas Jørgensen, Sander Bruun, and Michael Z. Hauschild

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Title:

Potentials for optimized production and use of biodiesel in a well-to-wheel study

- **Based on a comprehensive real-time LCA case study of multiple pathways**

Authors:

Ivan T. Herrmann[a,*], Andreas Jørgensen[a], Sander Bruun[b], and Michael Z. Hauschild[a]

*Correponding author: ivan.t.h.business@gmail.com; P: +45 22756975; F: +45 45933435

[a]Section of Quantitative Sustainability Assessment, Institute of Management Engineering, Technical University of Denmark, Produktionstorvet, Building 424, DK-2800, Kgs. Lyngby, Denmark

[b]Department of Agriculture and Ecology, Faculty of Life Sciences, University of Copenhagen, Thorvaldsensvej 40, DK.1871 Frederiksberg C, Denmark

Abstract

Background, aim, and scope.

The increasing awareness of environmental impact from petrochemical (PC) oil products, such as PC diesel, the continuously increasing price, and the depletion of PC oil are all reasons for the increased focus on alternative fuels, such as biodiesel. For this reason, the European Union has enacted a proposal which requires that each member state shall ensure that the share of energy from renewable sources in transport in 2020 is at least 10% of final consumption of energy (The European Parliament and the Council 2009). This LCA study assesses the environmental impacts from the production and use of biodiesel, as it is today (real-time), based on rapeseed oil and different types of alcohols using technologies that, are close to be or, are currently available. Different options for environmental improvement of production methods are evaluated.

Methods.

The functional unit is "*1000 km transportation for a standard passenger car*". All relevant process stages have been included, such as rapeseed production including carbon sequestration and N_2O balances and transportation of products used in the LCA. System expansion has been used to handle allocation issues.

Results and discussion.

The climate change potential from the production and use of biodiesel as it is today is found to be 57 kg CO_2-eq/1000 km while PC diesel is 214 kg CO_2-eq/1000 km. Options for improvement can be: increased use of residual straw from the rapeseed fields for combustion in a power plant where carbon sequestration is considered; change of the transesterficaiton process from a conventional process to an enzymatic process when using bioethanol instead of PC methanol. Results for land use, repiratory inorganics potential, human toxicity (carc) potential, ecotoxicity (freshwater) potential, and aquatic eutrophication (N) potential are also evaluated. Different sources for uncertainty are evaluated and the largest drivers for uncertainty are the assumptions embedded in the substitution effects. The results presented should not be interpreted as a blue print for an

increased production of biodiesel, but as a benchmarking point of the present and actual impact in a well-to-wheel (WTW) perspective of biodiesel *with* options for improving this production and use.

Conclusion and recommendations.

Based on the present analysis we recommend investigating further options and incentives for: increased use of rapeseed straw considering carbon sequestration issues; (from a climate change potential perspective) using bioalcohol instead of PC alcohol for the transesterification process.

Keywords: LCA, biodiesel, optimization, enzymatic/conventional transesterification.

1 Introduction

The European Union has enacted a proposal which requires that each member state shall ensure that the share of energy from renewable sources in transport in 2020 is at least 10% of final consumption of energy (The European Parliament and the Council 2009). It is expected that the total energy consumption for transport in 2020 will be 438.6 Mtoe (ec.europa.eu 2008). The production of biodiesel in Europe in 2008 was 5.5 million ton (Emerging-markets.com 2011).

As such the demand for energy from renewable sources is fixed and the main question that remains to be answered must be: *how to reach this target with the lowest possible environmental impact?*

This paper is based on a 3-years LCA research program. Two Danish companies, Emmelev A/S (emmelev.dk 2011) and Novozymes A/S (novozymes.com 2011), have been partners with focus on optimization of the environmental performance of biodiesel in a WTW perspective.

As a framework to handle this optimization problem, we use the optimization methodology outlined in Montgomery (2005) combined with LCA techniques. Different explanatory variables such as: transesterification processes, type of alcohol, and agriculture management system during our research, have been identified for production and use of biodiesel which potentially can give a better or worse response for the environmental impact categories. Other explanatory variables are presented in supporting information.

The initial project was focused on the transesterification process where either an enzymatic or conventional transesterification can be applied. The other explanatory variables were used for benchmarking the potential of the transesterification process with this explanatory variable.

Harding et al. (2008) develops a LCA of biodiesel production and compares enzymatic and conventional transesterfication process in a well-to-tank perspective with multiple impact categories and found that enzymatic biodiesel transesterification is environmentally advantageous compared to conventional biodiesel transestrificantion. Malça and Freire (2011) present a comprehensive review of 28 different LCA studies on biodiesel in Europe where all results are evaluated based on green house gasses (GHG) emissions per MJ. The two main issues raised in this review study are the variability of results and the different modeling approaches between the different LCAs. The different modeling approaches are explained by different assumptions regarding geographical scope, the functional unit, multifunctionality (i.e. allocation problems), and agricultural modeling (mainly N_2O-emissions). Other modeling differences are also mentioned which we regard as "prospective", i.e. answering the questions of what *can* happen, opposite to studies of "the current situation" which is based on observable processes. The GHG emissions are reported to be ranging from 15 to 170 kg CO_2-eq/GJ. According to Howarth et al. (2009) some, but few, biofuel studies reports on other environmental impacts than GHGs.

Our study addresses multiple environmental impacts including toxicity modeling based on the USEtox^{TM} methodology, nutrient balance calculations in the agricultural stage, land use and discuss the indirect land use change (ILUC) impacts. Production data is based on empirical data from a Danish biodiesel producer. The modeling is state-of-the-art of current production technology, which can be considered as a benchmarking point for improvement on the already established biodiesel production and use in Europe/Northern Europe. Furthermore, options for processes used in different biodiesel production steps which may reduce environmental impacts are investigated.

2 Materials and Methods

2.1 Goal Definition

The goal of this study is to present a full comparative and quantitative LCA of biodiesel from rapeseed oil in Northern Europe. Two baseline pathways (PW)s for benchmarking are developed: 1) the environmental impacts of production and use of biodiesel based on rapeseed oil, and 2) the environmental impact from production and use of PC diesel. Other pathways with alternative production technologies are developed for investigation of potential environmental improvements of biodiesel production and use in Northern Europe. This shall lead to a better and more informed decision support when making decisions about future activities for production and use of biodiesel.

2.2 Scope Definition

The LCA study addresses decision makers which are involved in direct production of biodiesel and decision makers which are developing policies for biofuels. The LCA is, as far as possible, based on current technologies. The functional unit for our system is 1000 km driving in a passenger diesel car with a 20 % blend of biodiesel (20B). The passenger diesel car is based on an Ecoinvent process (*Operation, passenger car, diesel, fleet average 2010/RER U*) which reflects a fleet average in Europe in 2010. The study includes tailpipe emissions, biodiesel production, oil production, alcohol production, and rapeseed production – including specific modeling of fertilizer and pesticide emissions. It is assumed in our study that biogenic CO_2 emissions to atmosphere is balanced out by an equal uptake of carbon by growing new crops in the production system (in the next time-period). Hence all biogenic CO_2 emission is accounted with zero impact while CO_2 emission origin from PC diesel is accounted as an increased CO_2 emission to the atmosphere. The product system is illustrated in Figure 1.

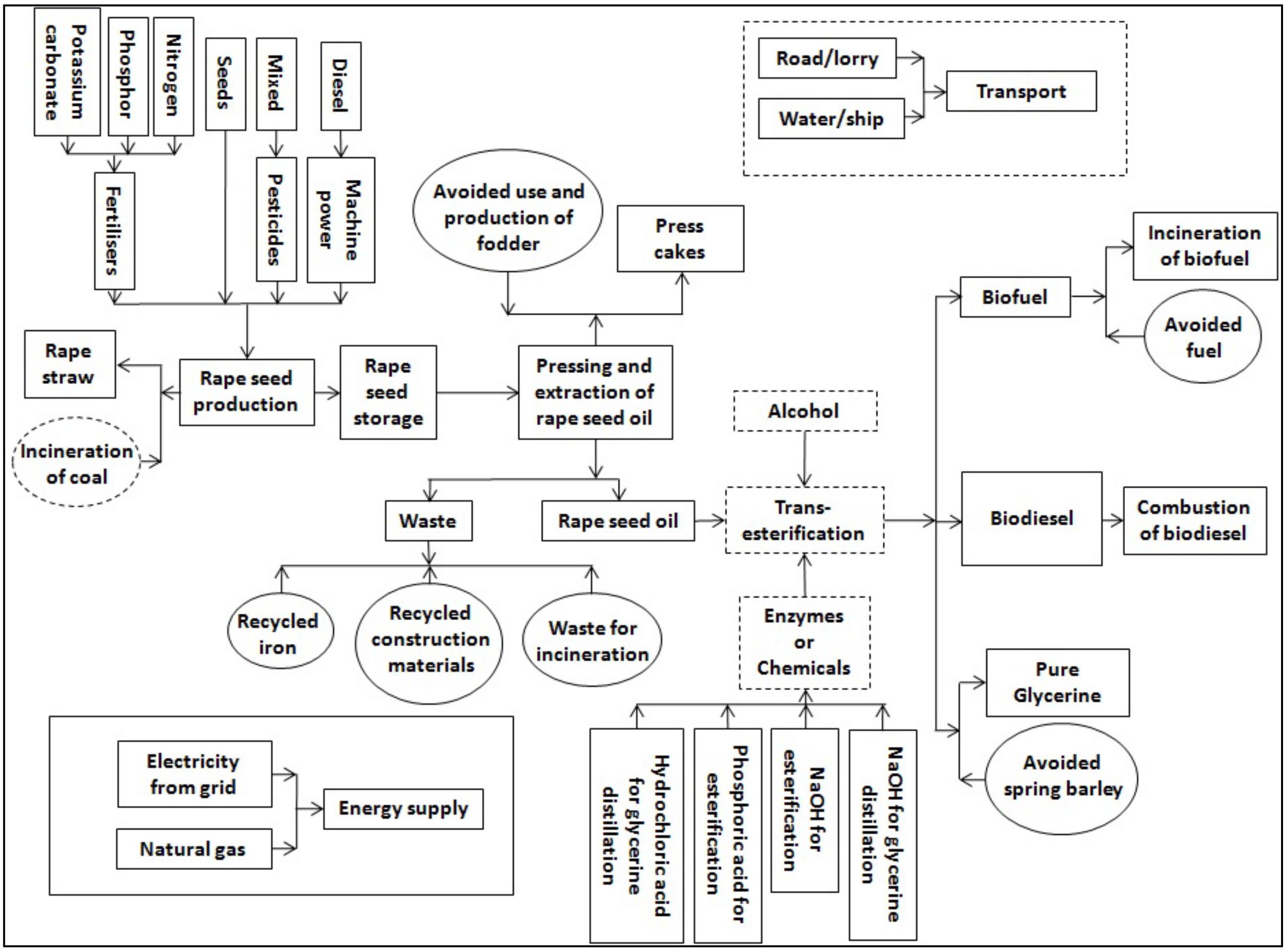

Figure 1 The analysed system for production and combustion of biodiesel for passenger car transport based on rape seed oil. Energy supplied for the pressing and oil extraction process and transesterification process is average Danish grid mix together with natural gas. Transportation includes road and water transport mainly for transport of seed to the pressing and extraction process. The dashed lines illustrate the variables that will or can be changed for creating alternative pathways (PWA2-8) – see table 1.

The choices that we have modeled based on Figure 1 are outlined in the following. For the transesterification step the choice is between 1) “Enzymatic 1”, 2) “Enzymatic 2”, and 3) a conventional transesterification process. For the alcohol production step the choice is between 1) PC methanol, 2) PC ethanol, or 3) bioethanol. For the agricultural step, the choice is 1) continue using the same amount of residual straw, as is used at present, for power generation in a power plant, 2) using an increased amount of rapeseed straw compared to present, or 3) not to use straw for power generation. For the transport the choice is between 1) short transport distance (local), or 2) long transport distance (regional). Different combinations of these options we regards as different PWs. However, at present not all of the combinations are technically possible or economically feasible, but they might still be interesting for further policy development or research.

Based on these choices, it is possible to make 3*3*3*2 = 54 different combinations. We have chosen to present two baseline PWs (PWD0 and PWA1) and seven alternative pathways for comparison with these baselines in this paper (PWA2-8). These pathways are outlined in Table 1. In table 1 the following abbreviations are used: *D = PC diesel*, *A = rapeseed* and each ID-number is used to identify the unique combination.

Table 1 shows the different pathways for biodiesel production and use which are discussed in this paper. *PW = pathways, D = PC diesel, A = rapeseed* and each ID-number is used to identify the unique combination. PWD0 and PWA1 are both considered as real baselines because they are today’s real production and use. I = 0 t/(ha*year), II = 0.52 t/(ha*year), and III = 0.86 t/(ha*year).

	Biodiesel production step			
Name	**Alcohol production**	**Transesterification**	**Agriculture**	**Transport**
PWD0	No	No	I	No
PWA1	PC Methanol	Conventional	II	Short
PWA2	Bioethanol	Conventional	II	Short
PWA3	Bioethanol	Enzymatic 1	II	Short
PWA4	PC Methanol	Enzymatic 2	II	Short
PWA5	PC Ethanol	Conventional	II	Short
PWA6	PC Methanol	Conventional	III	Short
PWA7	PC Methanol	Conventional	I	Short
PWA8	PC Methanol	Conventional	I	Long

The data for this LCA has been collected in the years 2009-2011. Based on Makridakis (1998) the modeling conducted in the present paper of PWD0 and PWA1 is addressing the time period of t_P = present (~ 2010). Data for PWD0 and PWA1 reflects average production data in Denmark[1] as it is

[1] When data for the present time period was limited, then assumptions were made to fit data to this criterion.

today (real-time). Hence no assumptions about what will happen in the future are made for these data or what will happen if production is *increased*. Forecasting of PWD0 and PWA1 is done by the "naïve forecast method" (Makridakis 1998) which is assuming that the best forecast for the future is the current value of the time series, given the information that was available during our research. This also implies that our study is not strictly comparable to the study of Edwards et al. (2008) since they are addressing potential environmental impacts from an *increased* production.

System expansion was used to solve allocation problems whenever allocation problems arose in our system. The system expansion has been based on literature surveys and specialist knowledge and product substitution was modeled, the way it is believed to be currently. We believe that system expansion is preferable to other methods for solving allocation problems, such as allocation based on mass or energy. Bernesson, Nilsson & Hansson (2004) illustrates and discuss the difference between the different allocation methods.

As a point of departure the EDIP2003 was chosen as the primary impact assessment methodology. However, not all of the presented impact categories were available in EDIP2003. Hence other methodologies were used primarily based on the criteria that they should be the newest available. The environmental impacts are evaluated based on the following six impact categories:

1. Climate change potential based on EDIP 2003 (Wenzel, Hauschild & Alting 1997)
2. Land use based on Recipe (Goedkoop et al. 2008) and Impact 2002+ (Jolliet et al. 2003)
3. Respiratory inorganics based on (Humbert et al. 2011)
4. Human toxicity (carc) based on USEtox^{TM} (Rosenbaum et al. 2008)
5. Ecotoxicity freshwater based on USEtox^{TM} (Rosenbaum et al. 2008)
6. Aquatic acidification (N) based on EDIP2003 (Wenzel, Hauschild & Alting 1997)

The study is based on data from a biodiesel producer in Denmark, technical research from Copenhagen University, and from DTU Chemical Engineering Department (Nordblad 15. June 2011). Other data has been found in the literature and remaining data is from the Ecoinvent database. All assumptions and all data are cited in the following lifecycle inventory (LCI) subsections. However, some of the data applied is classified and cannot be published, due to the projects stakeholder's business opportunities. The environmental modeling tool SimaPro (pre.nl 2011) (version 7.2) has been used including the EcoInvent database version 2.0.

2.2.1 Rapeseed production

The unit process “rapeseed production” models the emissions from rapeseed production under average Danish conditions. The process has been scaled to 1 ha*year.

The emissions of different nutrients from 1 ha*year agricultural oilseed rape field are calculated using nutrient balances of two different farm types (plant and pig) and two different soil types (sandy loam) and coarse sandy soil (according to Danish standards). Subsequently the emissions were averaged across the different groups by using the relative frequency of plant farms, pig farms, on coarse sandy soil, and sandy loam soil in Denmark (Table 2).

Table 2 Relative frequency of plant farms, pig farms, on coarse sandy soil, and sandy loam soil in Denmark (Knudsen 1st of October 2010)

	Coase sandy soil	**Sandy loam**
Pig Farms	0.25	0.41
Plant Farms	0.18	0.16

Nitrogen balances

For each of the four combinations of soil types and farm types, a nitrogen balance were calculated (Figure 2). There are two major inputs of nitrogen to the field one from nitrogen fertilizers and one from atmospheric deposition. The major outputs are removal of seeds and straw, ammonia volatilization, denitrification in form of N_2O and N_2 and nitrate leaching.

Fertilizer input was assumed to be in accordance with the Danish fertilizer norms (Naturerhvervsstyrelsen 2010) for oilseed rape i.e. 119 kg N ha^{-1} on the coarse sandy soil and 183 kg N ha^{-1} on the sandy loam. The plant farms are assumed to be fertilized with mineral fertilizer exclusively while the pig farms are assumed to be fertilized with pig slurry. A mineral fertilizer equivalency of 75% was assumed for pig slurry. Crop N uptake was estimated as the normative values (Naturerhvervsstyrelsen 2010). Emissions of N_2O and N_2, from fertilizer use have been based on the “SIMDEN” model (Vinther, Hansen 2004). Nitrate leaching was calculated from the nitrogen balance. The manure fertilizer is assumed to have zero climate change impact since it is considered to be a waste product from the pig production. Detailed description of nitrogen balance is available in supporting information.

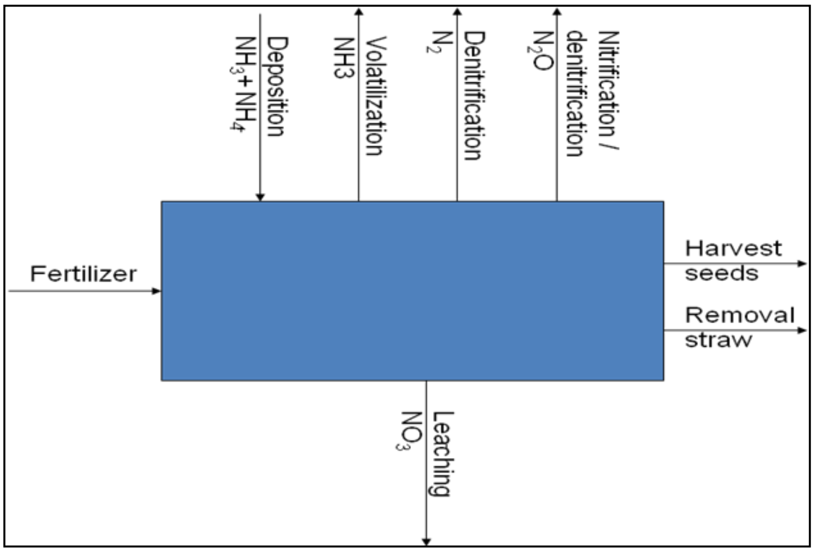

Figure 2. Model for nitrogen balance.

Phosphorous

The amount of mineral P applied on the plant farms was assumed to follow the Danish recommendations (Haastrup 2010). On the pig farms, P supply was assumed to supply ample and no mineral P was needed. The amount of P supplied was calculated from the amount of N supplied with slurry and a P to N ratio of 0.11 (Møller et al. 2001). The loss of P varies a lot depending on soil and manure type and climate, but we have no data to quantify this. Instead a gross average of losses to surface waters estimated to be 0.15 kg/ha by Munkholm and Sibbesen (1997) was used and other losses were assumed to be minimal. The rest of the P is either removed with the crop or accumulated in the field.

Potassium

The amount of mineral K applied on the plant farms was assumed to follow the Danish recommendations (Haastrup 2010). On the pig farms, ample K was assumed to be supplied from the animal manure and no mineral K was necessary. The losses og K were not estimated because losses of K are considered to have no impact on the environment.

Use of pesticides

In supporting information pesticides allowed for rapeseed cultivating in Denmark and the amount allowed to use of each pesticide according to (Danish Agro 2008) is presented. These doses we assume have been used to the full extent. To calculate emissions, the PEST-LCI (Birkved, Hauschild 2006) model has been used.

Use of rapeseed straw

Removing straw from the fields and use those for combustion in a power plant and consequently substitute coal can potentially improve the environmental impacts of biodiesel. However, removing too much straw from the field can lead to a risk of soil organic carbon mining. According to Lafond et al. (2009) it is possible to remove wheat straw from the field, without a change in the soil organic carbon (SOC), if no more than 40 % is removed in 2 out of 3 years (on average 26.7 % p.a.). Nor will there be a change in the yield of the spring wheat grain or the grain protein content. It is assumed that these results can be transferred to the production of rapeseeds. According to (dst.dk 2011) on average the production of rapeseed straw, between 2006 and 2009, was ~ 3.22 t (ha*year) resulting in a theoretical possible removal of mass of 0.86 t/(ha*year). However only 0.66 t/(ha*year) is removed according to dst.dk (2011) and of this 0.52 t/(ha*year) was used for incineration.

It can be assumed that there will be an approximately 3 % energy loss of the straw due to a required pre-treatment before they can be co-fired with hard coal in a power plant (Sander 3rd of Marts, 2010). With energy value of 14.5 GJ/t of straw the amount of coal, measured in GJ, which can be substituted is:

14.5 GJ/(t of straw) * 0.52 t/(ha*year)*0.97 (GJ from Coal/GJ from straw) ~ 7.3 GJ/(ha*year). If we use all the straw for incineration, which according to our calculations can be used safely, i.e. 0.86 t/(ha*year), then this can substitute coal incineration worth 12.12 GJ/(ha*year).

The emissions from burning rapeseed straw and coal in a power plant are practically equal due to the modern cleaning technology applied in Danish power plants (Karsten Hedegaard Jensen, Thyø & Wenzel 2007). The improvement is then mainly the change in carbon dioxide, carbon monoxide, and to a smaller extent methane emission, that will be biogenic instead of being from fossil resources.

2.2.2 Pressing and extraction of rapeseeds oil

The unit process "pressing and extraction of rapeseeds oil" has been scaled to 1 t of rapeseed input. According to lcafood.dk database (2006) the production of rapeseed meal is determined by the demand for the rape seed oil. The co-production of 1 t rapeseed meal from the rapeseed oil production substitutes soy meal production and barley for animal food with 0.664 t and 0.279 t (lcafood.dk database 2006).

2.2.3 Biodiesel production

The unit process "production of biodiesel" has been scaled to 1 t of rapeseed oil as an input. The major inputs for this process are: chemicals (or enzymes), energy, alcohol, and oil. In the case of conventional transesterification process the input data are based on production information from Emmelev A/S.

Two different enzymatic processes have been modeled, "Enzymatic 1" based on stoichiometry data from (Nordblad 15. June 2011) and "Enzymatic 2" based on Sotoft et al. (2010). The required input of enzymes has been based on data from Novozymes A/S. The environmental impacts for 1 kg of enzymes in a cradle-to-gate perspective are based on Nielsen, Oxenboll & Wenzel (2007). Both the Enzymatic 1 and Enzymatic 2 process are based on immobilized enzyme catalysts. Other enzyme processes, including those based on liquid formulated enzyme, could lead to somewhat different results.

Three different types of alcohol have been modeled, 1) PC methanol, 2) PC ethanol, and 3) bioethanol. The alcohols have all been modeled using standard processes from the Ecoinvent database. The by-products glycerine and biofuel are presented separately in subsection 2.2.5.

2.2.4 Combustion of biodiesel

The emissions from driving 1000 km in a diesel passenger car is based on the unit process "*Operation, passenger car, diesel, fleet average 2010/RER U*" which includes airborne emissions of gaseous substances, particulate matters and heavy metals. These data have been altered with biodiesel tailpipe emission data from the Graboski et al. (2003) report, which is based on test data of a "DDC Series 60 Diesel Engine". Emission from biodiesel per brake horsepower*hour (bhp-h) delivered at the axle is known which also is known relative to PC diesel. Assuming that the efficiency of the specific car does not change due to a change in the fuel type emissions from biodiesel, and then emissions from 1000 km delivered can then be deduced.

The biodiesel needed for driving 1000 km has also been calculated relatively to the Ecoinvent PC diesel process. In this unit process, it is estimated that 0.055828 t of PC diesel is consumed per 1000 km. The calorific energy value for PC diesel is 43.38 GJ/t (iea.org 2005) and for fatty acid methyl ester FAME it is 37.362 GJ/t. Test data from Graboski et al. (2003) shows that there is a small decrease in efficiency (for the specific test engine) of the PC diesel and biodiesel (7219btu/bhp-h)/(7433btu/bhp-h) ~ 3%. To deliver 1000 km from the biodiesel 0.0668 t biodiesel is needed. Table 3 shows the changes in emissions from biodiesel (20B) relative to PC diesel.

Table 3 Relative change in emissions based on Graboski et al. (2003) test data. The changes in emissions are measured per bhp-h delivered at axie. THC = total hydrocarbons. It is assumed that the change from FAME to fatty acid ethyl ester (FAEE) will result in the same relative change compared to PC diesel.

	THC	NOx	CO	CO_2	PM	SO_2	VOC
Cert Fuel (PC diesel)	1	1	1	1	1	1	1
FAME (Rapeseed)	1.05	1.00	0.86	1.00	0.83	0.80	0.82

To account for the different types of alcohol's contribution to the GHG's it has been assumed that the average length of the fatty acid carbon chains are ~ 17 C long, based on (Mattson, Volpenhein 1963). Adding methanol or ethanol to this will increase the length of the carbon chain with 1 respectively 2 carbon atoms. Adding bioethanol is accounted for in the tailpipe emission as being biogenic. The three different ratios applied in this study are then:

- (19 biogenic)/(19 total) for bioethanol (FAEE)
- (17 biogenic + 2 fossil)/(19 total) for ethanol from fossil resources (FAEE)
- (17 biogenic + 1 fossil)/(18 total) for methanol from fossil resources (FAME)

2.2.5 Glycerine and biofuel as by-products

There are two by-products from the biodiesel production process, namely crude glycerol and impure biodiesel. With the conventional transesterification process the crude glycerol is in PWA1 purified, which requires use of chemicals and energy. 2-3 % of the fuel output is considered to be too impure to meet the specifications that are required to serve as biodiesel. Instead it can be used in an industrial furnace where it is assumed to substitute light or heavy PC fuel oil where the energy value is 2-3 % lower than the pure biodiesel. Based on (Zijlstra et al. 2009) we assume that the glycerine can substitute wheat for feed for pigs. According to (Jonasson, Sandén 2004) it can be assumed that the substitution ratio between wheat and glycerine is ~ 0.93 kg wheat/(kg glycerine).

2.2.6 Transportation

The rapeseed transportation is going from a local farmer to the biodiesel producer with an average transport distance by lorry of 100 km. Some of the rapeseeds are from a regional farmer where transportation is by ship with an average distance of roughly 1000 km and 200 km with a lorry. These distances are considered relevant for the case since the Danish producer either uses local domestic rapeseed production or uses rapeseeds produced in Eastern Europe.

3 Results and discussion

In the following six figures each impact category are presented for each of the 9 PWs. For these results no emissions from indirect land use change (ILUC) are included. Results addressing ILUC are presented separately. Each PW is separated into two parts, tailpipe impact (Tailpipe) and production system impact (Production). At the top of each graph the aggregated number for both the tailpipe and the production is presented per 1000 km. In general we consider PWD0 and PWA1 as the production and use as it is currently, while the rest of the PWs are modeled with changes which, we think, are interesting to consider for improved production and use of biodiesel.

3.1 Climate change potential

PWD0, PC diesel, is the PW with the highest climate change potential, 214 kg CO_2-eq/1000 km. The tailpipe emission for PWD0 is approximately 180 kg CO_2-eq/1000 km while the PWA1 has a tailpipe emission of ~ 12 kg CO_2-eq/1000 km. The production stage level for PWD0 accounts for ~ 34 kg CO_2-eq/1000 km.

The production stage level for PWA1 accounts for ~ 45 kg CO_2-eq/1000 km. The change between PWA1 and PWA2 is that instead of using PC methanol then bioethanol is modeled. This leads to a decrease in the overall impact of ~ 9 kg CO_2-eq/1000 km due to a lower tailpipe emission. However, at present the conventional transesterification process based on ethanol is either technically possible (or economically feasible). The bioethanol is assumed to come from Brazil and transportation for this is included in PWA2. PWA3 is based on the enzymatic 1 transesterification process which makes it possible to use ethanol for the transesterification process. It can be seen that at present this process seems to be a little less efficient compared to the conventional process in PWA1. What is important to notice here is that the conventional transesterification process (PWA1) is a mature technology that has been developed over the last decades, while the enzymatic process is a new and rather immature technology. If the enzymatic processes are developed further, we would expect that there will be a higher potential for improving this technology compared to the already mature and conventional transesterification process. We have made no attempt to predict (or forecast) these potentials. This LCA study can serve as benchmarking for further improvement of both technologies. At least two variables can be used for further improvements of the enzymatic process. These are 1) the mass of enzyme needed per mass of biodiesel out, and 2) the CO_2-eq/t of enzyme produced.

PWA4 is based on Sotoft et al. (2010). PWA4 increases with 2 kg CO_2-eq/1000 km compared to PWA1 which is due to a slightly less efficient transesterification process. However energy data was not transparent from the Sotoft et al. (2010) paper and hence energy data has been roughly estimated.

PWA6-7 is similar to PWA1 except change in the amounts of straw which is used for incineration. PWA6 is, compared to PWA1, modeled with an increased mass of 0.34 t rape straw used for incineration in power plants which is assumed to substitute coal resulting in a decrease of 26 kg CO_2-eq/1000 km. PWA7 is modeled without any incineration of rape straw, which results in an increase of 42 kg CO_2-eq/1000 km compared to PWA1. PWA8 is modeled without incineration of rape straw but using a longer transportation distance (from Eastern Europe to Northern Europe by ship) of the rapeseeds which results in an increase of 10 kg CO_2-eq/1000 km compared to PWA7.

It should be noted that from Figure 3 other combinations are possible to construct than the ones that are presented. For example, if the gains of increased rape straw incineration in PWA6 are added to PWA2 then the overall impact would decrease even further to ~ 22 kg CO_2-eq/1000 km.

Our results are slightly different from the findings in Harding et al. (2008). This difference mainly origins from a rather high climate change potential of the chemicals used for the conventional transesterification process applied compared to the climate change potential from chemicals in the conventional transesterification process that we have applied. However, other differences might also explain the different results between our enzymatic and conventional transesterification processes and the results that Harding et al. (2008) presents. Furthermore, Harding et al. (2008) arrives at a result ranging from ~ 147 to 162 kg CO_2-eq/GJ in tank[2]. No incineration of straw is modeled in Harding et al. (2008). PWA1 has climate change potential of ~ 18 kg CO_2-eq/GJ in tank. The low heat value (LHV) used in Harding et al. (2008) is 27.1 GJ/t of biodiesel which seems to be a low estimate compared to Mehta and Anand (2009) findings of ~37-38 GJ/t of biodiesel which is our assumed efficiency, too.

[2] In tank refers to the accumulated impact in a well-to-tank perspective.

The climate change impact potential for our system seems to be in alignment with Edwards et al. (2008). Edwards et al. (2008) reports an upper quartile value of ~ 69 kg CO_2-eq/GJ in tank, a medium value of ~ 49 kg CO_2-eq/GJ in tank and a lower quartile value of ~ 25 kg CO_2-eq/GJ in tank. No incineration of straw is reported which can explain some of the observed differences. It should be noted that Edwards et al. (2008) addresses a possible increased production, and hence Edwards et al. (2008) results are not strictly comparable with our study in the sense that when modeling different scopes then also different results should be expected. For example, Edwards et al. (2008) assumes that some of the increased rapeseed production will be placed on lower quality land than the already established which then will result in a lower efficiency compared to our study. Bernesson, Nilsson & Hansson (2004) arrives at similar results ranging from ~ 30 to 88 kg CO_2-eq/GJ in tank. This range is explained by different allocation methods, where the system expansion is in the lower part of this range going from 30 to 35 kg CO_2-eq/GJ in tank. No incineration of straw is reported in Bernesson, Nilsson & Hansson (2004).

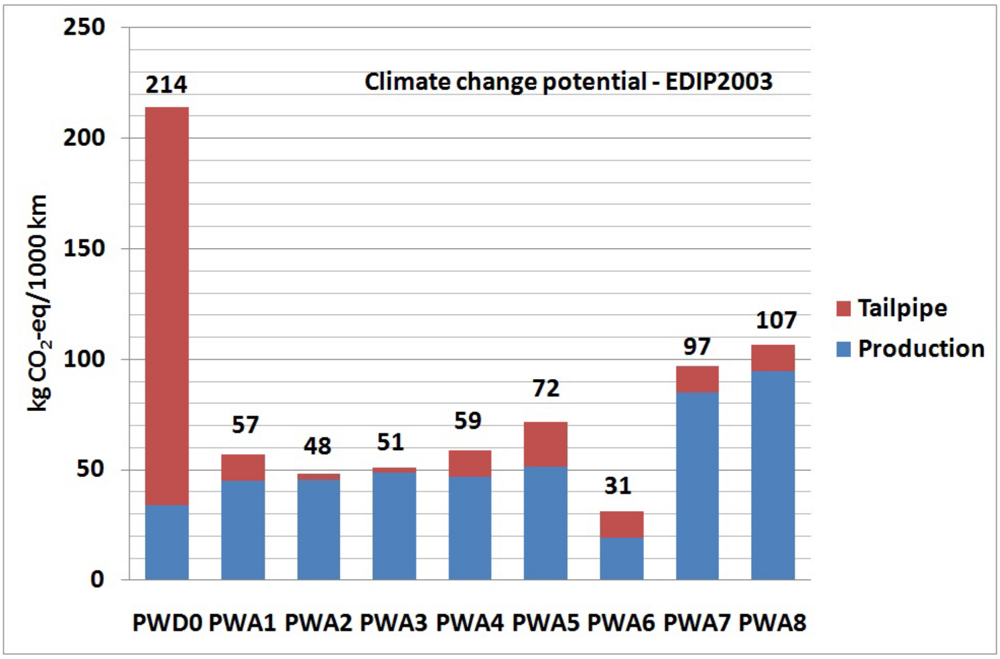

Figure 3. Climate change potential per 1000 km driven in a standard diesel passenger car - EDIP2003.

3.2 Land use

The land use impact category has been modeled based on the land occupied directly by the crop needed for driving 1000 km. For validation of the results, two different impact methodologies were chosen, namely Recipe and Impact2002+. It seems that for the different biodiesel PWs, the Recipe estimates are in general ~ 5 m^2a/1000 km smaller than the Impacts2002+ impacts. This difference we assume is a result of differences in the modeling principles in the two impact methodologies. The PWD0 differs quite a lot between the two impact methodologies (a factor of 2), but for comparison with the biodiesel PWs this problem is negligible as the absolute land use values for PC diesel are very small compared to PWA1-8.

The comparison between the different PWs reveals what should be expected. PWA2+3 have the highest land use impact which is due to land use from both the crop production for oil and the alcohol (bioethanol). PWA5 has a lower land use impact than PWA1 due to the larger alcohol molecule which results in slightly better land use efficiency of FAEE compared to FAME. Change in the use of rape straw and transportation, which is reflected in PWA6-8, does not change the overall land use impact.

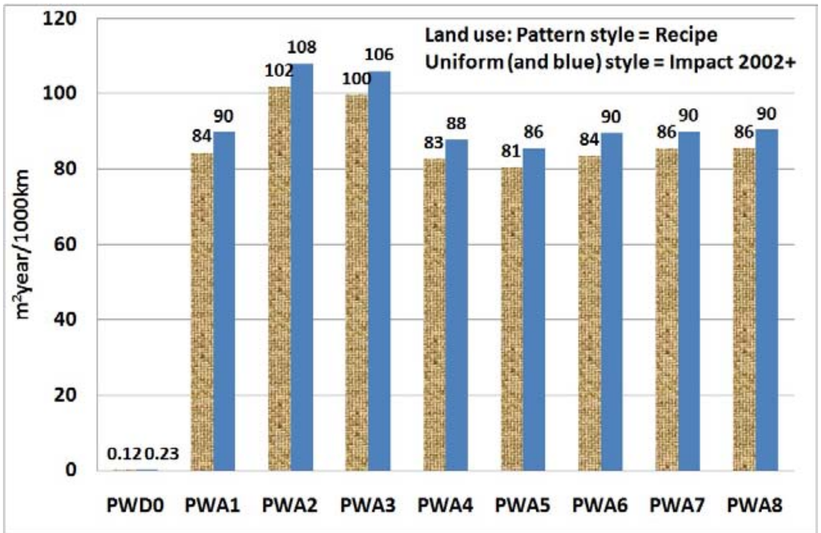

Figure 4. Land use based on Impact 2002+ and Recipe.

3.3 Respiratory inorganics potential

The human health impacts from respiratory inorganics have been modeled based on (Humbert et al. 2011). In general the total emissions for the PWA's are lower than for PWD0. For PWD0 ~ ½ of the emissions are from tailpipe while the other ½ is from production. PWA1 has almost ½ the 2.5 PM-eq. emission compared to PWD0. Approximately ¾ of the emissions in PWA1 is from tailpipe emissions. The tailpipe emissions are quite similar to each other across the PWA's and hence the difference between the impacts reflects differences in emissions from the production methods. PWA2+3 have both bioethanol as alcohol input to the transesterification process. The respiratory inorganics environmental impact from production of bioethanol is higher compared to production of methanol which is due to traction and transportation and production of the used fertilizers in the sugar cane production system. The larger impact from PWA8 compared to PWA1 is explained by the increased transportation of rapeseeds from Eastern Europe to Northern Europe. The overall impact of using PC methanol (PWA1) instead of using PC ethanol (PAW5) seems to be marginally better regarding the respiratory impact category. By increasing the use of straws (PWA6) we also see a slightly improvement in the respiratory inorganics impact category compared to PWA1, this improvement origins from reduced production of coal.

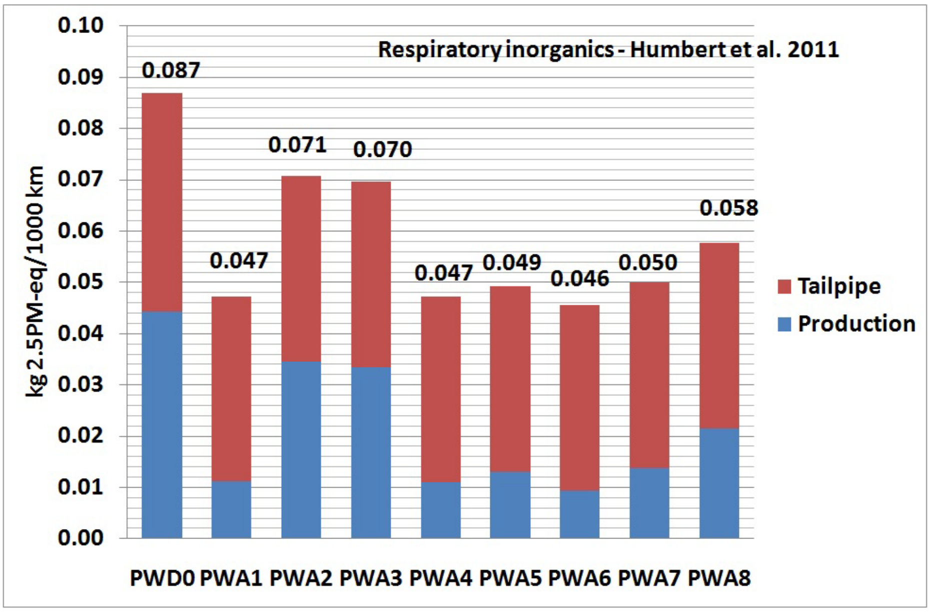

Figure 5. Repiratory inorganics - (Humbert et al. 2011).

3.4 Human toxicity (carc) potential

The human toxicity (carc) is modeled based on the USEtox^{TM} methodology (Rosenbaum et al. 2008); (Hauschild et al. 2008). The tailpipe emissions from PWD0 and PWA1-8 do not differ much. The major contribution to the human toxicity (HT) impact category is from production of nitrogen, production of phosphor, production of potassium carbonate which all are used for cultivating of rapeseed, and traction in the rapeseed production system. The main change in the emissions between the different pathways is to be found in the production systems. In general production of PC diesel results in less HT than from the biodiesel PWs. It can be seen from Figure 6, that the two bioethanol PW's (PWA2+3) have a higher HT impact compared to PWA1. PWA(3+4) indicates that the enzymatic transesterification process is preferable compared to the conventional transesterification process (PWA1+2). Changing the alcohol from PC methanol (PWA1) to PC ethanol (PWA5) will result in a higher HT impact. Increasing the use of rapeseed straw from the rapeseed field (PWA6) can potentially lower the environmental impact compared to (PWA1), which is also confirmed from PWA7 where a slightly higher HT impact is observed due to the change in extraction of coal. From PWA8 it can be observed that additional transportation in the production system increases the impact.

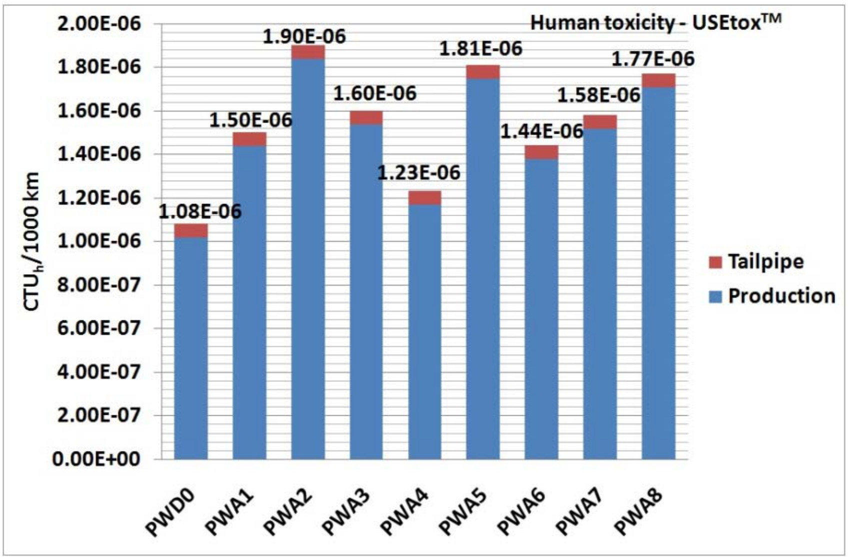

Figure 6. Human toxicity - USEtox$^{TM.}$. CTU_h = comparative toxic unit, human.

3.5 Ecotoxicity – freshwater potential

The ecotoxicity freshwater is modeled based on the USEtox™ methodology (Rosenbaum et al. 2008); (Hauschild et al. 2008). The major difference in the freshwater ecotoxicity impact observed between PWD0 and PWA1-8 is due to the difference in the production system. Small changes between biodiesel PWA1-8 can be observed. PWA6 results in an improvement of the ecotoxicity impact compared to PWA1, which is due to the reduced production of coal. The origin of this impact comes almost entirely from the use of pesticides in the rapeseed production.

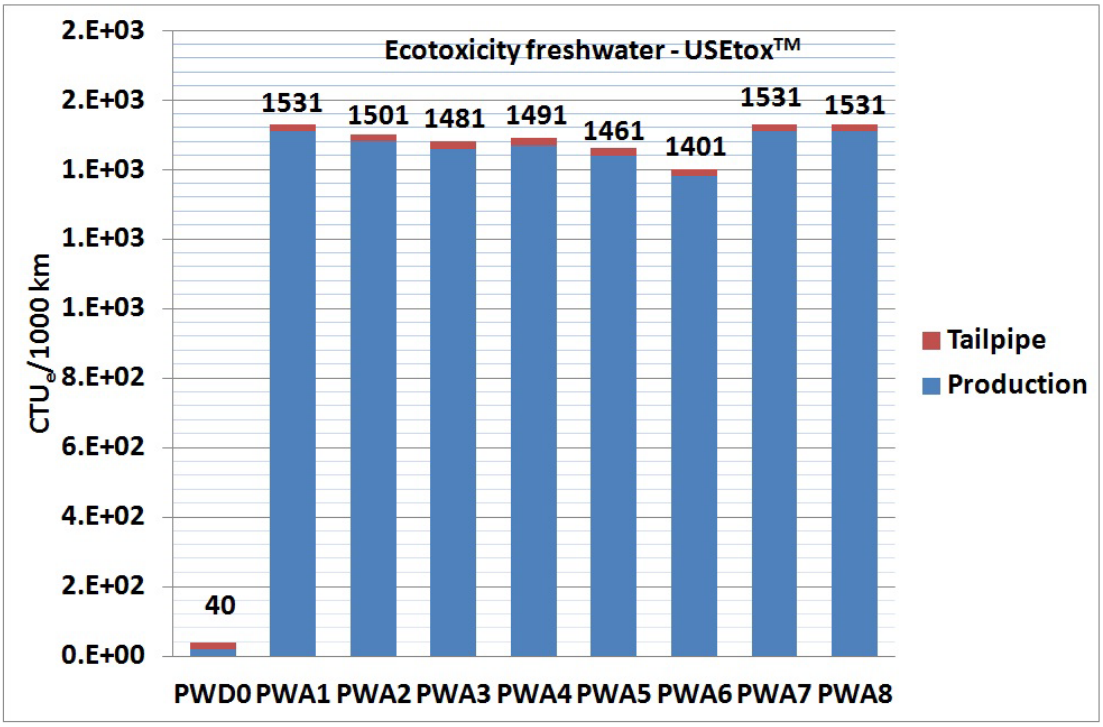

Figure 7 Ecotoxcity freshwater by USEtox™.

3.6 Aquatic eutrophication (N) potential

The aquatic eutrophication is modeled based on the EDIP 2003 methodology (Wenzel, Hauschild & Alting 1997). The major difference in the aquatic eutrophication impact observed between PWD0 and PWA1-8 is due to the difference in the production system. Small changes between the different biodiesel PWA1-8 can be observed. PWA8 has the highest impact due to an increased transportation compared to PWA1. The origin of this impact comes mainly from the rapeseed production system with contribution parts from the use of fertilizers and traction.

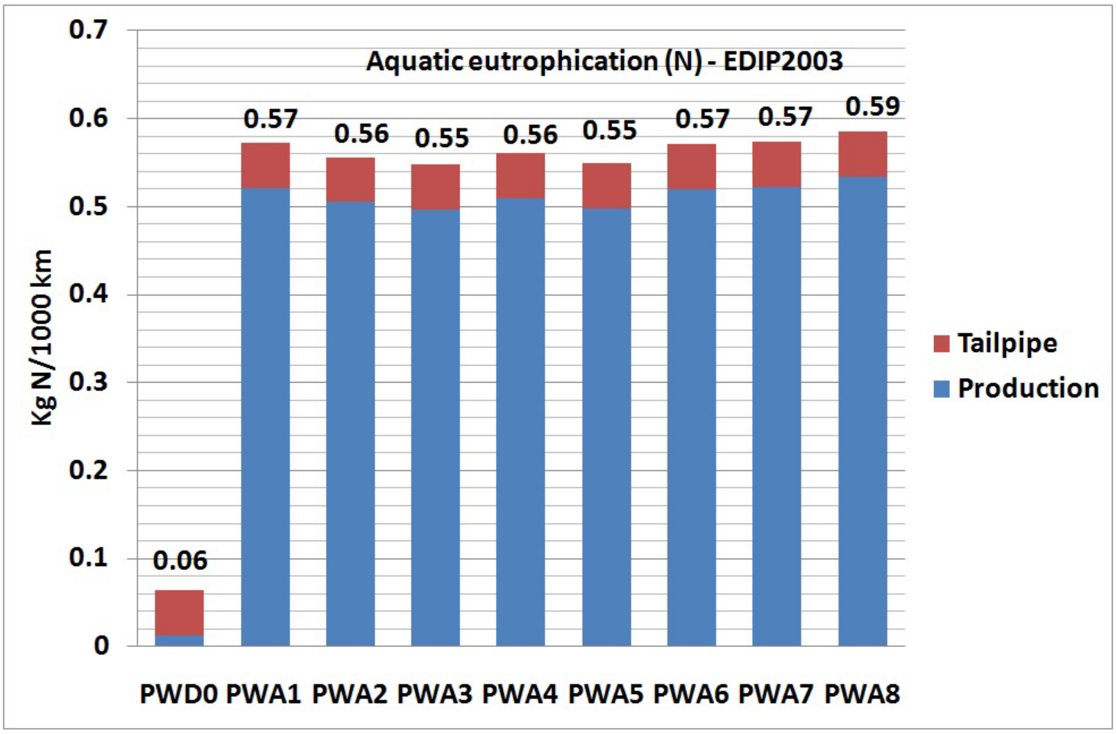

Figure 8. Aquatic eutrophication (N) using EDIP2003.

3.7 Uncertainty consideration

As pointed out by Mathiesen, Münster & Fruergaard (2009) substitution effects are not certain. In the present assessment, there are uncertainties related to the way system expansion has been carried out in order to solve allocation problems. As an example, it has been assumed that glycerol will substitute wheat in our study. According to Malça, Freire (2011) bio-glycerol can also substitute other products, such as PC glycerol. In Pagliaro (2010) other products, which glycerol can substitute, are discussed. Most of these are relevant for future time-periods (prospective) and not in the current time-period, which we are addressing. Based on these references and sensitivity runs in SimaPro, different substitutions can vary the impact potentials from different categories' with up to 10-15 %.

The different alternatives, PWA2-8, have been modeled with changes in the setup compared to PWA1. This means that the uncertainty of the impacts *between* the different PWAs is relative low. Since the presented LCA is comparable to a "still picture" of the present situation, other market effects than the system expansion used to solve the allocation problems are not modeled, such as rebound effects from increased production or increased efficiency. For example Mulalic (2011) shows that efficiency improvement of truck engines can lead to an (overall) increase in fuel consumption due to rebound effects. Another factor that can influence the uncertainty when modeling market effects, and hence substitution effects, is if the market is increasing or decreasing. If the market is increasing, it is plausible that no substitution effect will take place. The product that was assumed to substitute another product simply becomes an *additional* product on the market. In general, as discussed in Møller (1996) if changes are considered on a macro scale, then changes in the price vector should be considered, too.

3.7.1 Impact from indirect land use change

Based on Indirect Land Use Change (ILUC) numbers from Croezen et al. (2010) and energy values for rapeseed oils from Mehta and Anand (2009), impact from ILUC can be added to GHG's emissions in PWA1. A "medium ILUC impact", based on these numbers, will give an increased emission of ~ 107 kg CO_2-eq./1000 km, whereas a "high ILUC impact" of will give an increased emission of ~ 173 kg CO_2-eq./1000 km. However, our study addresses an established production of biodiesel as it is today. The study is not addressing what can happen if the production of biodiesel is increased prospectively. The available ILUC numbers are addressing what can happen, as an indirect effect, if rapeseed production is increased. This means that a distinction between these two

LCA scopes is important for the interpretation of the results and what the results can be used for. This concern is also reflected by Halleux et al. (2008). The results in the present paper should not be interpreted as a blue print for increased biodiesel production. The results represent options for improvements of the already established production. Furthermore and as extensively discussed by Gawel and Ludwig (2011) there are several uncertainty issues with ILUC numbers that would need some attention before they are applied. Two of these issues mentioned are causality and how to measure the ILUC impact. Regarding causality, it can be difficult to distinguish different drivers for land use change from each other. Kline and Dale (2008) list other possible drivers (such as: cultural-, technological-, biophysical- and economic forces) than a single crop market to be a driver for land use changes. Measuring or monitoring these different drivers is problematic. For example, data used in the Global Trade Analysis Project (GTAP)[3] model is based on voluntary reporting and data that can be rather old, such as Swedish Input-Output data from 1985 (Reinvang, Peters 2008).

[3] The GTAP model is used to calculate ILUC impacts according to Hedal, Baltzer & Nielsen (2010).

4 Conclusion

Six different impact categories have been evaluated in this study in a WTW perspective. The main sources for the environmental impact are summarized in the following and options for improvements are suggested.

In PWD0 the main source for climate change potential origins from the tailpipe emission with a tailpipe/(production + tailpipe)-ratio of 180/214 kg CO_2-eq./1000 km (~ 84 %). The impact from PWD0 is used to benchmark the findings for PWA1-8.

Climate change potential: For the different biodiesel pathways the main impacts comes from the agricultural stage where especially the use of mineral fertilizer (ammonium nitrate), traction for harvesting and transport of rapeseeds contributes to the climate change potential. Potential for significant improvements of this production system comes from increased use of rapeseed straws for incineration which is assumed to substitute coal and lower transportation in the product system. Bioethanol or biomethanol can be used to reduce the tailpipe emission compared to PC ethanol or methanol.

Land use: PWD0 represents an insignificant use of land compared to PWA1-8. Using bioethanol compared to PC ethanol (or methanol) will increase the land use ~ 15-20 %. If it is desired to decrease land use then PC alcohol (and/or oil) is favorable.

Repiratory inorganics potential: PWD0 has the largest respiratory inorganics impact potential. Among PWA1-8 the PWA2+3 have the highest impacts due the use of bioethanol.

Human toxicity (carc) potential: The lowest impact is from PWD0. Between the different PWA1-8 there is some variation. The main sources origins by far from the production stage both for the PC diesel and the biodiesel. For PWA1-8 the largest contribution origin from the use of fertilizer. It is not preferable to change alcohol from PC methanol to bioethanol with regard to human toxicity potential.

Ecotoxicity – freshwater potential: The PWD0 has, by far, the lowest impact. PWA1-8 have more or less similar impacts. All most all the impacts come from the production system. The origin of this impact comes almost entirely from the use of pesticides in the rapeseed production.

Aquatic eutrophication (N) potential: The major difference in the aquatic eutrophication impact observed between PWD0 and PWA1-8 is due to the difference in the production system. Small changes between the different PWA1-8 can be observed. The origin of this impact comes mainly from the rapeseed production system with contribution parts from traction and the use of fertilizers.

4.1 Recommendation and perspectives

Based on the present analysis we recommend investigating further options and incentives for:

- Increased use of rapeseed straws taken problems of carbon sequestration into consideration.
- From a climate change potential perspective using bio-alcohol instead of PC alcohol in the transesterification process.
- From a climate change potential perspective changing the fuel used in the system from PC fuel to biofuel.
- From a land use perspective using PC diesel instead of biodiesel.

5 Acknowledgement

We would like to thank Alexis Laurent for implementing the Humbert et al. (2011) methodology into SimaPro and letting us use it. We would also like to thank the editors and the reviewers for helpful comments. Funding was provided by Technical University of Denmark, Novozymes, and The Danish National Advanced Technology Foundation which we are very grateful for.

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SUPPORTING INFORMATION

Title: **Potentials for optimized production and use of biodiesel in a well-to-wheel study**

\- Based on a comprehensive real-time LCA case study of multiple pathways

Journal: The International Journal of Life Cycle Assessment

Authors:

Ivan T. Herrmann[a,*], Andreas Jørgensen[a], Sander Bruun[b], and Michael Z. Hauschild[a]

*Correponding author: ivan.t.h.business@gmail.com; P: +45 22756975; F:+45 45933435

[a]Institute of Management Engineering, Section of Quantitative Sustainability Assessment, Technical University of Denmark, DK-2800, Produktionstorvet building 424, Kgs. Lyngby, Denmark

[b]Department of Agriculture and Ecology, Faculty of Life Sciences, University of Copenhagen, Thorvaldsensvej 40, DK.1871 Frederiksberg C, Denmark

1 Nitrogen balance

The fertilizer input of nitrogen is based on the nitrogen norms defined for the specific soil type in Danish regulations (Naturerhvervsstyrelsen, 2010). In these regulations the “mineral fertilizer equivalencies” (MFE) for different types of fertilizers are also defined. For mineral fertilizer this is 100% and for pig slurry it is 75%. Based on the norm and the MFE, the amount of N added as fertilizer can be calculated.

For pig slurry, the amount of ammonia volatilization was calculated from a standard value for application with a trailing hose of 10.5% of the applied ammonia (Sommer and Hutchings, 2001) and an estimate of the fraction of N in pig slurry that is ammonium is 75%. No volatilization is assumed to occur.

Nitrogen deposition is assumed to be 13 kg/ha which is a gross average for Denmark (Ellermann et al., 2010). Denitrification and the fraction of this which is N_2O is calculated using the SimDen model (Vinther and Hansen, 2004) for the particular soil type and fertilizer applications in the different cases.

The harvest of oilseeds was based on the yield norms for the specific soil type (Naturerhvervsstyrelsen, 2010). From this and a protein content from fodder tables and an N content in proteins of 16%, the amount of N in the harvested oilseeds are calculated. Similarly, the amount of N removed with straw is calculated from the average amount of straw removed (dst.dk 2011) and an average content of N of 0.6% (Holmes 1980). Finally, leaching was calculated by assuming the there is no accumulation of N in the field.

2 Use of pesticides

Table S1 summarizes the data used to calculate emissions of pesticides. In the reference system the first number corresponds to the columns and second number to the rows. Total weight per ha:

2.095 kg/(ha*year) of active ingredients. The quantification and modeling of the emission has been done by applying the PEST-LCI model (Birkved, Hauschild 2006).

Table S1. List of pesticides used for improved agriculture output in Danish rapeseed production.

Table of pesticides used in cultivating rapeseeds						
(0.0)	**1**	**2**	**3**	**4**	**5**	**6**
1	**Name of Pesticide**	**Dose [kg or L/ha]**	**Active ingredients**	**Conc. Of active ing. [g/L]**	**Active ing. [g/ha]**	**CAS no and Ecoinvent**
2						
3	**Autumn**					
4	Command CS	0.27L	Clomazone	360	97.2	81777-89-1
5	Fastac 50	0.2L	alpha-cypermethrin	50	10	67375-30-80
6	Ferramol	5.25kg	ferrifosfat	0.099 % (w/w)	52.5	10045-86-0
7	Focus Ultra (+ Dash)	0.5L (+ 0.5L)	Cycloxydim	100	50	101205-02-1
8	Cantus	0.35kg	Boscalid	50 % (w/w)	175	188425-85-6
9	Mangansulphat (+ Dash)	2kg + (0.15L)	Mangan	319,8 g/kg	640	
10						

11	**Spring**					
12	Kerb 500 SC ~ has been taken of the market					
13	Focus Ultra (+ Dash)	0.5L (+ 0.5L)	Cycloxydim	100	50	101205-02-1
14	Matrigon	0.8L	Clopyralid	100	80	1702-17-6
15	Solubor	4.5kg	Bor	175 g/kg	787.5	
16	Biscaya	0.25L	thiacloprid	240	60	111988-49-9
17	Fastac 50	0.25L	alpha-cypermethrin	50	12.5	67375-30-80
18	Folicur EC 250 + Amistar	0.5L + 0.25L	Tebuconazol + azoxystrobin	250 + 250	125 + 62.5	107534-96-3/ 131860-33-8

In the reference system the first number correspond to the columns and second number to the rows.

(1,1): Information from ” Planteværn 2008 Markjournal” (reference 1 – see below)

(2,1): Information from ”Planteværn 2008 Markjournal” (reference 1 – see below)

(3,1): Middeldatabasen.dk (2010) (reference 2 – see below)

(4,1): Middeldatabasen.dk (2010) (reference 2 – see below)

(1,7), (1,9), and (1,13): Dash: Solvent naphtha (naphthalene depleted); CAS# 64742-94-5 33-37% (w/w) - Fedtsyrer, C16-18- og C18-umættede, menthylestere; CAS# 67762-38-3; (w/w) 36-39% - Fettalkohol, ethoxyliert, Phosphorsauree, CAS# 68649-29-6; 18-20% - Phosphorsyre; CAS# 7664-38-2; 3-4%. (Dash - agro.basf.dk 2010) According to (Dash - middeldatabasen.dk 2010) the density of Dash is 1000g/, however additives, in general, are without any significant biological impact why Dash is not included in the toxicity assessment.

(3,6) - the Ferric Phosphate in general do no harm according to www.epa.gov (2010) and it is assumed it is not necessary to include this ingredient for toxicity purpose.

(3,9) og (3,15) the Manganese and Boron is not used for pesticide purpose. These ingredients are used because the crop is short of these minerals. In this assessment it is assumed that 20 % of these minerals are not up taken by the crop and are for this reason emitted to air, soil, and water.

(3,8) – Boscalid has not to be found in the available database through SimaPro. However according to www.epa.gov (2010) this pesticide is relative harmless. It has therefore been assumed to be safe to leave out this pesticide from the assessment.

(3,16) - Thiacloprid was not to be found in the available database through SimaPro.The best possible alternative to this ingredient is estimated to be Imidacloprid which is from the same group of pesticides - Neonicotinoids – and is the most commonly used of these according to wiki (2010).

For the ingredients that are not marked have not been able to model using PEST-LCI because these ingredients is not a part of the database in the present version. Based on the ingredients that are available in the database an average ratio of the flows to water, air, and soil have been calculated.

3 Other explanatory variables than presented in the paper

In the following some additional explanatory variables are outlined. These variables can either increase or decrease the environmental impact from biodiesel production and use.

Feedstock: Chicken fat, soybean, palm oil, algae oils, jatropha oil are all oils which can be used for production of biodiesel.

Regions: Different regions that produce biodiesel can explain differences in response parameters. This can be explained by different energy supplies with a higher or lower degree of coal, hydropower, and nuclear power etc. in the grid mix. Also different types of climate will potential could affect the efficiency of the production of the biodiesel.

Cars/engine and emission/cleaning technologies: Different types of engine or car technologies can either increase or decrease the environmental impact for use of the biodiesel.

Substitutions of other products: Which kind of products that are substituted can also be used as explanatory variables.

4 References

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Appendix C: Does it matter which LCA tool you choose?

- Comparative assessment of SimaPro and GaBi on a biodiesel case study

Authors: Ivan T. Herrmann, Andreas Jørgensen, Morten Birkved, and Michael Z. Hauschild

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Ivan T. Herrmann*, Andreas Jørgensen, Morten Birkved, and Michael Z. Hauschild
Institute of Management Engineering, Section of Quantitative Sustainability Assessment, Technical University of Denmark, Produktionstorvet, building 426, DK-2800, Kgs. Lyngby, Denmark

*Corresponding author: ivan.t.h.business@gmail.com
P: +45 22756975
F: +45 45933435

Title: **Does it matter which LCA tool you choose?**

Subtitle: **- comparative assessment of SimaPro and GaBi on a biodiesel case study**

1 Abstract

Goal, Scope, and Background.

SimaPro and GaBi are two of the leading software tools used for life cycle assessments. In this paper, their performance is compared based on an applied case study of biodiesel. The research question is; can there be a difference between using SimaPro and GaBi, influencing the results and conclusions of the LCA study and the decisions based on it?

Methods.

The two programs' performance is compared following a 4 step approach; 1) comparison of inventories obtained from GaBi respectively SimaPro based on an identical biodiesel product system; 2) Investigation of some of the differences observed between SimaPro and GaBi in the first step; 3) Comparison of a standard unit process (i.e. "of-the-shelf" EcoInvent unit process) which has identical inventory in SimaPro and GaBi. Comparison performed at the level of characterization-, normalization-, and weighting using three LCIA methodologies, EDIP2003, CML 2001, and Eco-indicator 99; 4) Comparison of aggregated impact potentials obtained for the biodiesel product system.

Results and Discussion.

A clear difference is observed for the inventories calculated for the biodiesel product system with SimaPro and GaBi. A maximum ratio of a factor 10 between the obtained inventory results is observed for the air-borne emission of 2,3,7,8 – TCDD (dioxin). Most of the inventory differences observed are caused by differences in the implementation of a single EcoInvent unit process on hydrochloric acid. Comparing the inventories obtained from SimaPro and GaBi for this process results in a maximum ratio of a factor 1380. Also the implementation of the impact assessment methodologies shows considerable differences. For the same life cycle inventory the maximum ratio for the characterized values is 1160 for abiotic depletion calculated with the CML 2001 methodology. Finally, for the aggregated impact potentials obtained for biodiesel product system, the difference between SimaPro and GaBi was observed to be a ratio 12. The observed differences seem to come mainly from errors in applied databases for both inventory and impact assessment.

Conclusion and recommendations.

SimaPro and GaBi are used by many LCA practitioners worldwide as a decision support tool, and if the results of the present analysis are just suggestive for the differences in the results obtained when using one or the other of the programs, then the implications of this paper are worrying. It is clearly in the interest of both software developers and LCA practitioners that the observed differences are addressed in the future development of LCA decision supporting tools, e.g. through ring tests comparing the tools.

Keywords: SimaPro, GaBi, Comparative Assessment, LCA Software, Biodiesel.

2 Introduction

With the increasing focus on sustainability issues the life cycle assessment (LCA) methodology is increasingly being used for quantitative evaluation of environmental impacts caused by products, services, and technologies. Two of the leading software tools used for LCA studies are SimaPro (pre.nl 2012) and GaBi (pe-international.com 2012), both applied worldwide. For the LCA practitioners looking for advanced software tools that can assist in performing a quantitative environmental LCA a natural question is “does it matter which software I choose?” It is the purpose of this paper to investigate this question.

GaBi is a LCA software that came on the market in 1992. It is developed and distributed worldwide by PE INTERNATIONAL, a German company (pe-international.com 2012). SimaPro is a LCA software that first was released in 1990 and likewise since then sold worldwide. It is developed and distributed by PRé Consultants, a company based in the Netherlands (pre.nl 2012).

Both software include; a) a user interface for modeling the product system, b) a life cycle unit process database, c) an impact assessment database with data for several impact assessment methodologies, d) an interface for analysis, and e) a calculator that combines numbers from the databases in accordance with the modeling of the product system in the user interface. To get a more detailed description of the two software we refer to the manuals of the two programs (pre.nl 2012 and pe-international.com 2012).

3 Method

In this analysis four different product systems or sub systems are used for comparing SimaPro and GaBi. The four systems are; 1) Own Biodiesel Model (OBM), 2) Non-aggregated Unit Process (NUP), 3), Aggregated Unit Process (AUP)[1], and 4) aggregated Soybean at Brazilian Farm (SBF)[2]. The last one is a specific item from the AUP population but to ease the reading of the present text a distinction is made between the SBF and the rest of the AUPs.

An initial comparison of the two tools is based on the product system modeled in the OBM, an LCI study of biodiesel based on rape seed oil produced in Denmark. The OBM product system is a well-to-wheel system documented in Herrmann et al. (2012) and briefly illustrated in section 4 "Biodiesel from a well-to-wheel perspective". The exact same OBM product system was modeled in both software tools so it was possible to compare the results of the two software for the exact same system of processes. The procedure for modeling the OBM product system in SimaPro and GaBi and the comparison of the results obtained with the two software are described in the following.

First it was ensured that the versions of GaBi and SimaPro used in the comparison were the newest versions available when the study started and that both were fully updated and the unit process databases were identical. The GaBi version used was: 4.4.101.1 (Compilation); DB version 4.131 including the EcoInvent database version 2.01. The SimaPro version used was: 7.2.4 Faculty; Database version 2.0. The EcoInvent help desk assured that this database version was the same as 2.01 (lca-net.com 5. November 2010).

Since then, updates have been made available for both software. These updates could potentially influence the results which this paper is based on if a similar comparison were to be conducted today. However, due to the speed of the research, paper writing, and the submission process compared to the speed with which new software updates are coming, it is not possible to make a comparison based on software versions that are also the most recent when the paper is published. This is a limitation of the analysis. However, given that the assessment is made at a random point in time, and that it is made for two relatively mature software, where there is no guarantee that updates

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[1] When no abbreviation is used it can be either NUP or AUP

[2] All four systems are modelled based on the EcoInvent database.

will converge towards more similar results, it seems reasonable to make the comparison under the present conditions. Furthermore, a recheck of some of the important differences observed in the present paper was conducted based on two newer versions of Simapro (version 7.3.2 Faculty version) and GaBi (4.4.135.1). The findings from this recheck are placed in section 5.4.

Setting up the OBM gave some problems. One problem was the different handling of ‘avoided productions’ (in case of system expansion) and the handling of waste in the software. In GaBi the ‘avoided production’ is handled either by inverting a receiving process or by converting the by-product output into a negative demand. In SimaPro avoided production and waste is handled in a formalized way provided in the software.

Furthermore, SimaPro includes all upstream flows when using non-aggregated unit processes, NUPs, whereas this is not the case for GaBi. It was therefore ensured that all the processes used in the comparison were aggregated unit processes, AUPs to eliminate this source of error. Another difference between the two software tools is the difference in the numbers and types of environmental compartments to which emissions can occur. In some cases adjustments were thus needed before a comparison was possible. For freshwater, GaBi has one and only one compartment whereas in SimaPro emissions to the freshwater compartment can go into groundwater, river, lake, or unspecified freshwater. It was found through comparing characterization factors that the factors applied for freshwater emissions in GaBi equal the characterization factors applied for unspecified emissions to water in SimaPro. For emissions to soil, the same procedure was followed, and it was found that emissions to agricultural soil in GaBi matched emissions to agricultural soil in SimaPro, whereas emissions to industrial soil in GaBi corresponded to unspecific emissions to soil in SimaPro. When creating the OBM object in the two software these differences were considered.

Having created the OBM object in both software, a meticulous quality assuring procedure was performed to ensure that name and quantity for each AUP in SimaPro and GaBi matched exactly. This was done by copying and pasting the OBM objects from GaBi respectively SimaPro into a spreadsheet and by inventory comparison ensure that both names and quantities matched for each AUP. In cases where an AUP needed to be changed to create a new element, all flows in the AUP were also copied into the spreadsheet and compared in order to ensure a complete match. In this way it was ensured that the OBM objects built in the two software were the same, both in structure, in processes, and in quantities.

After having completed the implementation of the OBM object in both software tools, the quantitative comparison of the OBM object was conducted. This quantitative comparison was based on values from SimaPro inventory and GaBi inventory. Outputs from SimaPro respectively GaBi are in this paper called *output values* or just *values*. Output values for GaBi are denoted G and output values for SimaPro are denoted S.

For each elementary flow in the inventories, and for the characterized-, normalized-, or weighted indicator values from the two tools the S/G ratio was calculated. An S/G ratio of 1.00 is interpreted as "no difference" while anything else than 1.00 is interpreted as a difference. The larger the deviation of the ratio is from 1, the larger is the difference between the results of the two software.

A four step approach was followed in the comparison of SimaPro and GaBi. The four steps were:

A) Comparison of the two inventories for the OBM object obtained using SimaPro and GaBi
B) Analysis and tracking of sources for major result differences observed in step "A"
C) Comparison of the SBF object at the characterization-, normalization-, and weighting level
D) Comparison of aggregated impact potentials for the OBM object

A) Early in the comparison phase it became evident that a full comparison of the OBM object inventory lists from the two software was not practical due to the sheer number of output values (each list comprised 500-1000 flows) and in particular differences in names applied for the same elementary flows. Instead, three elementary flows with identical names in both software were selected for each impact category. These elementary flows were used consistently in all performed inventory comparisons.

B) Sources for differences at the inventory level were investigated to identify the main drivers behind the differences between SimaPro and GaBi found in step "A" for the OBM object.

C) For a comparison of the impact assessment of the two tools at the characterization-, normalization-, and weighting level, differences in the applied inventory had to be neutralized to be sure that any observed deviations between the results would be caused by differences in the performance of the impact assessment by the two tools. This was ensured by using the inventory for a unit process that was as close to identical as possible. Three EcoInvent AUPs were investigated as candidates: Soybean at Brazilian Farm (SBF), Rapeseed oil methyl ester and Spring barley. The inventory for the three candidates was tested for differences using the approach described under step "A". For the two latter AUPs there were considerable differences in the inventories despite the fact that they were supposed to be the same EcoInvent process. The test of the SBF object, on the other hand, showed only few differences on individual elementary flow level as well as for the sums for the total in- and output flows for mass (kg); energy (MJ); radioactivity (Bq); and area (m^2). The test of the SBF can be found in Supporting information, S4-5. For some of the impact assessment methods provided in the two software, different versions were stated. In these cases we decided not to perform a comparison. Only for LCIA methods where the version numbers were identical, or where no version number was stated for one or both software tools, we found it reasonable to assume that a practitioner using the software tools could assume that the impact assessment methods provided in the tools were equally up to date versions. These criterions disqualified impact assessment methods such as Impact 2002+ and Recipe. The impact assessment methodologies that were compared for the two software tools were EDIP2003 (Hauschild 1998), CML 2001 (cml.leiden.edu 2007), and Eco-indicator 99 (Goedkoop, Effting & Coltignon 2000). For CML 2001 the normalization and weighting step were not included since the reference year for the normalization step in GaBi was not indicated and there were no weighting factors available in SimaPro. For all three impact assessment methods we have only included the impact categories that were available in both software.

D) A final comparison of the aggregated environmental impact potentials (weighted and summed across impact categories) was conducted for the OBM object using EDIP2003 to see to how much potential errors would sum up to and how this could influence final decision support.

4 Biodiesel from a well-to-wheel perspective

The OBM object (Own Biodiesel Model) used for the first parts of the comparison of SimaPro and GaBi is based on an LCA study of biodiesel made from rapeseed oil by a Danish producer. The full LCA is documented in Herrmann et al. (2012). All data applied are representative for the production of biodiesel in 2009-2010 where the data were collected. Figure 1 illustrates the production system that has been modeled.

The biodiesel study is a well-to-wheel study with the functional unit of 1 MJ delivered for transportation with a diesel passenger car[3]. The product system has been modeled in four main life cycle stages 1) agricultural production of rapeseeds, 2) oil pressing and extraction, 3) transesterification process, and 4) combustion of biodiesel. The modeling of the agricultural production stage includes modeling of the nitrogen balance and carbon sequestration in the field, and incineration of approximately 20 % of the rapeseed straws in a cogeneration power plant with a consequential substitution of coal burned in the power plant. In the oil extraction stage press cakes from the oil mill are assumed to be used for fodder and substitute spring barley and soy bean. The main output from the transesterification process is biodiesel. However, a small fraction of the output is too impure to meet the specifications and cannot be used as diesel in an ordinary diesel engine. This fraction is termed “biofuel” and is used as a fuel for industrial heating where it is assumed to substitute petrochemical light fuel or heavy fuel. Glycerol, which is another by-product from the transesterification process, is used in fodder and thereby assumed to substitute spring barley. In the last stage, the combustion of biodiesel, the biodiesel is assumed to substitute petrochemical (PC) diesel in a 1MJ to 1MJ ratio.

[3] The functional unit has been rescaled from 1000 km transport to 1 MJ in the present paper.

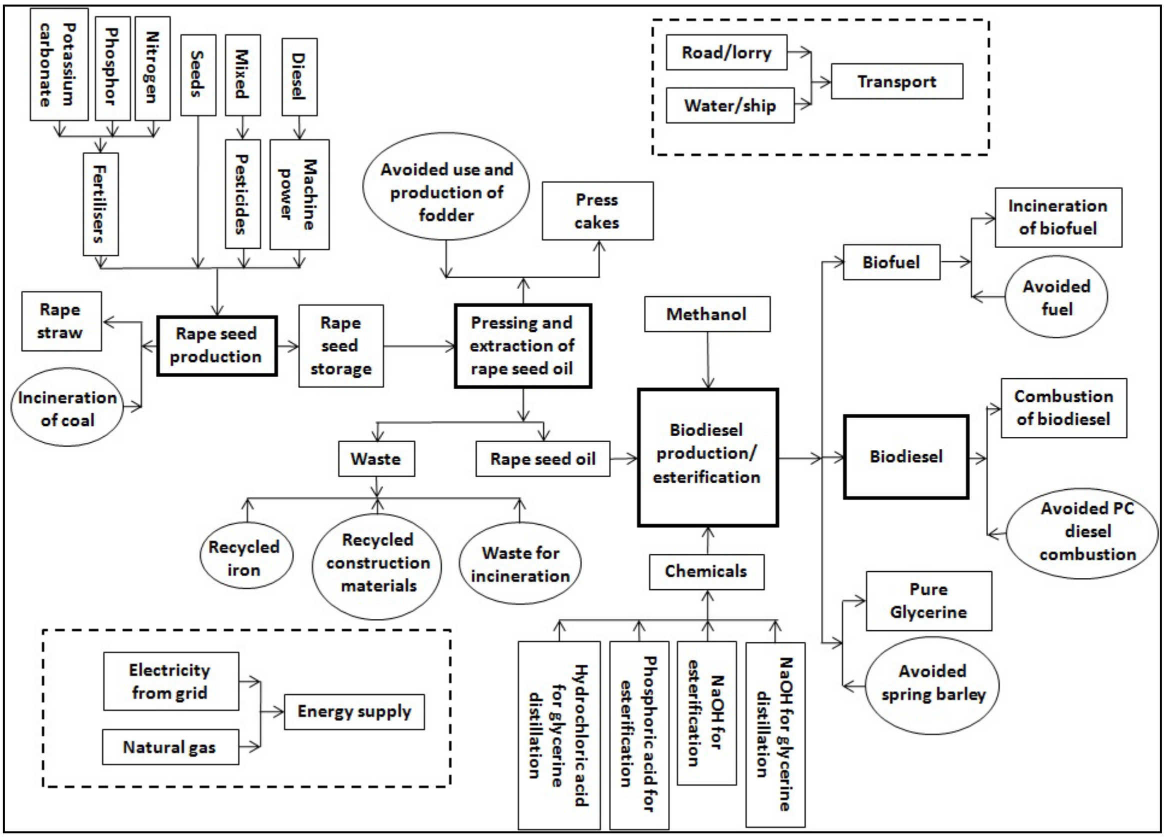

Figure 1. Production system in the OBM for production and combustion of 1 MJ of biodiesel for passenger car transport based on rape seed oil. Energy supplied for the pressing and oil extraction process and esterification process is average Danish grid mix together with natural gas. Transportation includes road and water transport mainly for transport of seed to the pressing and extraction process. PC = petrochemical (diesel).

5 Results and discussion of comparison of SimaPro and GaBi

The results of the comparisons at different levels and for different modeling objects are shown first for inventory and then for impact assessment applying different impact assessment methods implemented in the two software.

5.1 Comparison of inventories from SimaPro and GaBi for identical product system models

For the OBM object considerable differences were observed in the two inventories obtained from SimaPro and GaBi. For 14 out of the 39 selected flows the ratio between "S" and "G" was different from 1.00. Six of the 14 ratios were above 1.00 while eight were below 1.00. The maximum S/G ratio observed among the selected flows are 0.10 (corresponding to a factor 10) for 2,3,7,8 – TCDD. The results can be found in Table S1 in the Supporting information. One of the main sources behind the differences observed for the inventory comparison was found to be the process for production of hydrochloric acid. Table 1 shows the inventory for the hydrochloric acid process from SimaPro and Gabi for these 39 elementary flows and the ratios between these flows. The results for the OBM object excluding hydrochloric acid can be found in Table S2 in the Supporting information.

Table 1 is split into three main rows: Environmental impacts, Resource Consumption (RC), and Toxicological impacts (according to the categorization applied in GaBi). All output values are in kg or MJ. Furthermore, Table 1 is split into two main columns: Name of substance and specific compartment (e.g. air or soil). Table 1 shows considerable differences between the GaBi and SimaPro. Only two substances (Nitrate and Carbon tetrachloride) output value's results in an exact ratio of 1.00. CFC-11 and Hexane has the maximum ratio of a factor 1380 and 116. In addition some of the output values obtained from SimaPro are not available in GaBi or they are in GaBi estimated to be zero such as Tebuconazole.

It was investigated if the observed differences were rooted in a potential *swop* between the specific compartments which could be a likely explanation since SimaPro and GaBi operate with different emission compartments. If the aggregated output value across all emission compartments showed a ratio of 1 (or close to 1) and the ratio between the compartment specific emissions were different from 1, then swops between the different compartments could be a source for the observed differences in Table 1. However, the frequency of ratios of 1 was not higher among the ratios based on the aggregated emissions compared to the ratios based on compartment specific emissions. Some of the ratios for the aggregated emissions increased and some decreased compared to the output value for the specific compartments. It cannot be rejected that swops between the specific emission compartments take place but other sources are also needed to explain the observed differences. It has not been possible to track these sources further. Results for the aggregated output values for the AUP hydrochloric acid process can be found in Supporting information, Table S3.

Table 1. Inventory comparison of the AUP hydrochloric acid process obtained from EcoInvent.

IC	IP	Emission	Comp.	Comp. specific emissions		
				S (kg)	G (kg)	Ratio (S/G)
EI	AP	Nitrogen oxides	air	1.66E-03	1.62E-03	1.02
		Sulfur dioxide	air	3.03E-03	2.90E-03	1.05
		Hydrogen chloride	air	5.09E-05	3.75E-05	1.36
	GWP	Carbon dioxide	air	8.65E-01	7.36E-01	1.18
		Carbon monoxide	air	1.40E-03	6.26E-04	2.23
		Methane	air	1.70E-03	9.77E-04	1.73
	NEP	Phosphorus	water	4.63E-07	3.07E-07	1.51
		Nitrate	water	2.77E-04	2.76E-04	1.00
		Nitrous oxide (N2O)	air	2.37E-05	2.39E-05	0.99
	ODP	CFC-11	air	5.88E-13	4.26E-16	1380.38
		Carbon tetrachloride	air	1.10E-06	1.10E-06	1.00
		CFC-114	air	6.92E-09	4.34E-09	1.59
	POP (high)	Tetrafluoromethane	air	2.12E-07	3.73E-08	5.68
		Butane	air	5.96E-06	5.45E-06	1.09
		Benzene	air	3.64E-06	4.19E-06	0.87
	POP (low)	CFC-113	air	5.45E-11	0.00E+00	na.
		Butene	air	6.56E-08	7.08E-08	0.93
		Phenol	air	5.24E-08	6.75E-09	7.77
RC	-	Nitrogen in air/atmosphere	-	0.00E+00	0.00E+00	na.
		Crude Oil (in ground)	-	5.89E-02	6.04E-02	0.98
		Gravel/aggregate	-	1.09E-01	7.81E-02	1.40
TI	ES (chronic)	2,4-D	soil	3.14E-11	0.00E+00	na.
		Cadmium	soil	1.09E-09	1.55E-09	0.70
		Clomazone	soil	0.00E+00	0.00E+00	na.
	EW (acute)	Alpha-cypermethrin	water	0.00E+00	0.00E+00	na.
		Azoxystrobin	water	0.00E+00	0.00E+00	na.

		Lead/Lead(II)	water	9.22E-07	1.43E-06	0.64
	EW (chronic)	Clopyralid	water	0.00E+00	0.00E+00	na.
		Tebuconazole	water	2.77E-05	0.00E+00	na.
		Mercury/Mercury(II)	water	6.37E-08	5.99E-08	1.06
	HT(air)	2,3,7,8 - TCDD	air	4.29E-13	9.03E-11	0.00
		Hexane	air	3.19E-06	2.75E-08	115.78
		Antimony	air	4.39E-08	1.59E-08	2.77
	HT(soil)	Napropamide	soil	5.95E-12	3.66E-12	1.63
		Zinc/Zinc(II)	soil	3.46E-07	5.53E-07	0.63
		Nickel/Nickel (II)	soil	1.12E-08	4.73E-08	0.24
	HT(water)	Cumene	water	1.15E-07	2.07E-07	0.55
		Thallium	water	1.48E-08	1.00E-08	1.47
		Copper/Copper (II)	water	2.95E-06	1.06E-05	0.28

AP Acidification Potential, *Comp.* Compartment, *ES(chronic)* Ecotoxicity Soil chronic, *EW(acute)* Ecotoxicity water acute, *EW(chronic)* Ecotoxicity water chronic, *G* GaBi, *GWP* Global Warming Potential (GWP 100 years), *HT(air)* Human Toxicity air, *HT(soil)* Human Toxicity soil, *HT(water)* Human Toxicity water, *IP* Impact Potential, *NEP* Nutrient Enrichment Potential, *ODP* Ozone Depletion Potential, *POP(high)* Photochemical Ozone Fformation Potential (high NOx), *POP(low)* Photochemical Ozone Fformation Potential (low NOx), *RC* Resource Consumptions, *S* SimaPro, *soil* Agricultural soil and industrial soil, w*ater* Fresh water and sea water.

5.2 Comparison of characterized-, normalized-, and weighted results

We observed from "step A" that the two software tools do generate different inventory results for the OBM object. Consequently, in order to compare the impact assessment calculations in the two tools, the SBF object (Soybean at Brazilian Farm) was identified as an aggregated unit process with so modest differences in the inventory in the two tools that it could be used for investigation of potential differences between the performance of SimaPro and GaBi at the characterization-, normalization-, and weighting level. The functional unit for the SBF object was chosen to be 1 kg soybeans. The results from the comparison of the SBF inventories can be seen in Supporting information, S4-5.

Results from the comparison of the characterized-, normalized-, and weighted level using the impact assessment methods EDIP 2003, CML 2001, and Eco-indicator 99 are presented in Tables 2-

6. The comparison Tables have three main columns presenting the results at the characterized-, normalized-, and weighted level where possible. Each of the main columns is split into three sub-columns; an output value for SimaPro respectively GaBi and a column with the ratio between the two. From Tables 2, 4 and 5 quite different results are obtained for some of the impact categories from the two software tools. The differences vary between impact assessment methods, and are also dependent on the impact assessment step.

5.2.1 EDIP 2003 results

For the EDIP 2003 method the ratios between the characterized values in Table 2 obtained with the two tools deviate from 1.00, except for the categories Acidification and Terrestrial eutrophication. The highest observed ratios are 102 for Photochemical ozone formation (human exposure) and 6.18 for Global warming. The ratios observed between the characterized impact values are the same as for the normalized impact values, indicating that the normalization does not contribute to differences in the impact assessment results and hence seems to be implemented consistently in the two tools. An exception is the impact category Aquatic eutrophication, where a normalization value around a factor 5 larger is used in GaBi in comparison to SimaPro, hereby partially counteracting the bias introduced in the characterization. The weighting step with the default set of weighting factors introduces small changes in the ratios for most of the impact categories. Differences between the ratios relating to the normalization and weighting steps of around 10% are found in the two software for *both* Aquatic eutrophication and Photochemical ozone formation. Several smaller differences are found for the other impact categories, indicating that the EDIP2003 weighting step is not consistently implemented in the two tools. Overall the characterization step is the strongest contributor to the differences in impact assessment results. The underlying causes of the largest differences in this step for the impact categories Photochemical ozone formation (human) and Global warming are investigated further below.

Table 2. Comparison of characterized, normalized and weighted impact potentials for the SBF using the EDIP 2003 LCIA method.

	Characterized				Normalized			Weighted		
Impact category	Units	S	G	Ratio	S/(PE)	G/(PE)	Ratio	S/(Pt)	G/(Pt)	Ratio
Global warming 100a	kg CO_2 eq	1.68E+00	2.71E-01	6.18	1.93E-04	3.12E-05	6.18	2.12E-04	3.49E-05	6.07
Ozone depletion	kg CFC11 eq	1.38E-08	1.27E-08	1.08	1.34E-07	1.23E-07	1.08	8.42E-06	7.77E-06	1.08
Photochemical ozone formation (Vegetation)	m^2.ppm.h	1.37E+01	1.22E+01	1.12	9.82E-05	8.74E-05	1.12	1.18E-04	1.16E-04	1.01
Photochemical ozone formation (Human)	person.ppm.h	1.03E-03	1.01E-05	102	1.03E-04	1.01E-06	102	1.24E-04	1.35E-06	91.6
Acidification	m^2 UES	6.64E-02	6.64E-02	1.00	3.02E-05	3.02E-05	1.00	3.93E-05	3.83E-05	1.02
Terrestrial eutrophication	m^2 UES	2.07E-01	2.07E-01	1.00	9.84E-05	9.84E-05	1.00	1.18E-04	1.20E-04	0.98
Aquatic eutrophication EP(N)	kg N	5.92E-03	3.77E-02	0.16	4.93E-04	6.51E-04	0.76	6.91E-04	7.94E-04	0.87

SimaPro: EDIP 2003, version 1.02. GaBi: EDIP 2003, version of impact assessment method is not stated. *S* SimaPro, *G* GaBi, *PE* Person-equivalents, *Pt* PE-target emissions.

As can be seen in Table 2, the largest ratio is found for Photochemical ozone formation (human). The main reason for this seems to be a difference in the CFs applied in the two software. In Table 3 the CFs for some of the substances contributing to the Photochemical ozone formation (human) impact category are listed. A rather consistent ratio of a factor 1000, can be observed between the SimaPro and GaBi CFs, which could indicate that the CF values which are given in pers.ppm.h/g in Hauschild and Potting (2004) have been entered as if they were given per kg in GaBi. For 1-Propanol the ratio of 469 does not have an obvious explanation. The SimaPro values seem to be applied consistently (applying the efficiency factor for the group of alcohols as correction factor for 1-Propanol).

When the ratio between the total characterized Photochemical ozone formation impacts is less than the three orders of magnitude that is observed for individual substances in Table 3, it reflects that there are other contributing substances for which the difference is more modest or where there may be no difference so the inventory-weighted average across the impact category ends at a factor 102.

Table 3. Comparison of CFs substances contributing to photochemical ozone formation (POF). The names of the substances in the Table are the SimaPro names.

Substances	Unit	SimaPro	GaBi	Ratio
1-Butanol	Person.ppm.h/kg	5.900E-02	5.900E-05	1.00E+03
1-Butene	Person.ppm.h/kg	1.416E-01	1.300E-04	1.09E+03
1-Butene, 2-methyl-	Person.ppm.h/kg	1.121E-01	1.100E-04	1.02E+03
1-Butene, 3-methyl-	Person.ppm.h/kg	1.289E-01	1.200E-04	1.08E+03
1-Pentene	Person.ppm.h/kg	1.534E-01	1.500E-04	1.02E+03
1-Propanol	Person.ppm.h/kg	3.894E-02	8.300E-05	4.69E+02
1,2-Butanediol	Person.ppm.h/kg	4.425E-02	4.400E-05	1.01E+03

There is also a noticeable difference between SimaPro and GaBi regarding the characterized Global warming values. Investigation of the CFs for the emissions of biogenic and fossil carbon dioxide, carbon monoxide and methane shows a difference between how biogenic carbon is handled in the two tools. In SimaPro no CF values for inputs of carbon dioxide, outputs of biogenic carbon dioxide, and outputs of biogenic carbon monoxide are given. In GaBi on the other hand, the CF value is 1 for uptake carbon dioxide and 1 for the emission of biogenic carbon dioxide. Furthermore, emission of biogenic carbon monoxide has a CF value of 2. Similarly biogenic methane has a CF value of 20 in SimaPro, whereas in GaBi it is 25.

It could be argued that if an attributional LCA approach is followed, using mass allocation, then this difference between the handling of carbon will in most cases be insignificant. The reason is that in this case, the mass is conserved, meaning that input equals output. Hereby, the input of CO_2 in the growing of the rape equals the output of CO_2 when the rapeseed oil is burned as biodiesel in the car. In this case, whether CO_2 is given a CF of 1 for the uptake and 1 for the emission as biogenic CO_2 will give the same result as if both CFs were 0. However, the two software also differ in the handling of CO and CH_4, and these differences are bound to create some smaller differences in the results, simply because there is no uptake of CO or CH_4 to counterbalance the CFs of the emissions. The main problem is, however, that in most LCAs, there is no mass conservation, either because mass allocation is not used consistently or because the study is made after a consequential LCA methodology. Depending on the case, this may create significant differences in the input and output of CO_2-eq. and thereby result in significantly different Global warming results between SimaPro and GaBi.

5.2.2 Eco-indicator 99 results

For the Eco-indicator 99 method both the Egalitarian approach and the Hierarchist approach have been included in the comparison of SimaPro and GaBi. The individualist approach has not been included due to different version numbers in the two tools. The results for the Hierarchist approach are shown in Table 4. The ratios for the Egalitarian approach are shown in Supporting information, S6. They only differ from the results in Table 4, for Respiratory inorganics and fossil fuels where there are minor differences. The highest ratios observed in Table 4 for the characterized impact results are for the impact category Climate change with a ratio of 9.84 while Radiation has a ratio of 0.15 or nearly a factor 7 between the two tools. The difference in the Land use values may reside in a merger of the Land use category and the Land conversion category in SimaPro. The output values from GaBi are for Land use 2.39 PDF.m^2.yr and for Land conversion 5.06 PDF.m^2 respectively. With SimaPro there is only one output value regarding Land occupation, namely for Land use which is 7.74 PDF.m^2.yr which is close to the sum of the two GaBi values. In the SimaPro characterization factor database for the Eco-indicator 99 method there are only characterization factors for Land use. Land use and Land conversion cover different types of impacts and are expressed in different metrics. Merging the two categories and summing their results (in different metrics) appears as a flaw.

Whereas the ratios in Table 4 for the weighted results in all cases are equal to the ratios for the characterized values, the ratios for the normalized values are very different, and in many cases much higher. The reason for these somewhat peculiar normalized results is that the normalization and weighting are performed differently in the two software: In SimaPro there is only one normalization reference and one weighting factor for each of the damage categories; Human health, Ecosystem quality, and Resources. Thus, in SimaPro the normalization references and weighting factors are grouped. In GaBi a normalization and weighting factor is made uniquely for each impact category. The grouped normalization references used in SimaPro differ from the individual normalization references used in GaBi. This creates a difference between the ratios for the characterized and normalization results. After the weighting step these differences disappears because the product of the grouped normalization references and weighting factors used in SimaPro corresponds to the product of the individual normalization references and weighting factors used in GaBi.

Table 4. Comparison of characterized, normalized and weighted impact potentials for the SBF using the LCIA method Eco-indicator 99 – Hierarchist approach.

	Characterized				Normalized			Weighted		
Impact category	Units	S	G	Ratio	S (PE)	G (PE)	Ratio	S (Pt)	G (Pt)	Ratio
Carcinogens	DALY	9.76E-07	8.91E-07	1.10	6.35E-05	4.46E-04	0.14	2.54E-02	2.31E-02	1.10
Respiratory organics	DALY	6.21E-09	6.36E-09	0.98	4.04E-07	9.30E-05	0.00	1.62E-04	1.65E-04	0.98
Respiratory inorganics	DALY	3.56E-06	3.57E-06	1.00	2.32E-04	3.34E-04	0.69	9.27E-02	9.28E-02	1.00
Climate change	DALY	3.50E-07	3.56E-08	9.84	2.28E-05	1.49E-05	1.53	9.12E-03	9.24E-04	9.87
Radiation	DALY	4.64E-10	3.19E-09	0.15	3.02E-08	1.19E-04	0.00	1.21E-05	8.27E-05	0.15
Ozone layer	DALY	1.41E-11	1.41E-11	1.00	9.20E-10	6.45E-08	0.01	3.68E-07	3.67E-07	1.00
Ecotoxicity*	PDF.m^2.yr	3.81E-03*	3.66E-03	1.04	7.43E-07	4.51E-06	0.16	2.97E-04	2.85E-04	1.04
Acidification/ Eutrophication	PDF.m^2.yr	3.62E-02	3.61E-02	1.00	7.06E-06	9.62E-05	0.07	2.82E-03	2.81E-03	1.00
Land use	PDF.m^2.yr	7.7	2.39	3.24	1.51E-03	6.06E-04	2.49	6.04E-01	1.86E-01	3.24
Minerals	MJ surplus	1.00E-02	8.45E-03	1.18	1.19E-06	5.71E-05	0.02	2.38E-04	2.01E-04	1.18
Fossil fuels	MJ surplus	1.86E-01	1.56E-01	1.19	2.22E-05	1.89E-05	1.17	4.44E-03	3.72E-03	1.19
Land conversion	[PDF.m^2]	NA	5.06	NA	NA	1.28E-03	NA	NA	0.39E+00	NA

SimaPro: Eco-indicator 99, v 2.07 nov. 2009. GaBi: Eco indicator 99, version not stated. Acronyms: *S* SimaPro, *G* GaBi, *NA* Not Available, *PE* Person-equivalents, *Pt* PE-target emissions, *PDF* Potentially Disappeared Fraction of species, *DALY* , Disability Adjusted Life Years.
*Results from SimaPro in PAF.m^2.yr converted to PDF.m^2.yr by multiplication with 0.1 PDF/PAF according to Larsen and Hauschild (2007).

5.2.3 CML 2001 results

SimaPro and GaBi apply different normalization reference versions for the normalization step in the CML 2001 methodology and no weighting factors are given in SimaPro. Hence, it was only meaningful to compare the characterized step for the CML 2001 methodology. The characterized results obtained for the SBF object are presented in Table 5. The extreme ratio between the characterized values observed for Abiotic depletion with more than three orders of magnitude is most likely due to the division of the Abiotic depletion impact category in GaBi into one relating to resources and one relating to fossil fuels. What is compared is therefore the ‘full’ Abiotic depletion result from SimaPro with a ‘subset’ of the Abiotic depletion result in GaBi. We have not possible to compare the 'full' result from both software, as the Abiotic depletion result related to fossil fuels in SimaPro comes in Sb-eq. while in GaBi it comes in MJ-eq. The negative ratio for Global warming is explained by different CFs for handling the input of carbon and the emission of biogenic carbon in SimaPro and GaBi as discussed in Section 5.2.1 for the EDIP 2003 impact assessment results. The ratios of the Ecotoxicity values are for both Freshwater and Marine ecotoxicity around a factor 5 but in opposite directions, i.e. SimaPro has a Freshwater ecotoxicity 5 times higher than GaBi, while the opposite is the case for Marine ecotoxicity. The main reason for the difference with regards to Fresh water ecotoxicity is that emissions of heavy metals to water, especially nickel ion, have different characterization factors in GaBi and SimaPro. This difference is only found when including long term effects in SimaPro, which is the default setting in the software, but given that it is the 'infinite' Fresh water aquatic ecotoxicity we are looking for, as indicated in the Table below, they seemed necessary to include. The main reason for the higher result on Marine aquatic ecotoxicity in GaBi was that the CF for emissions of hydrogen fluoride to air is around a factor 80 higher in GaBi than in SimaPro.

Table 5. Comparison of characterized impact potentials for the SBF using the CML 2001 LCIA method.

	Characterized			
Impact category	Units	S	G	Ratio
Abiotic depletion	kg Sb eq	7.75E-04	6.68E-07	1.16E+03
Acidification	kg SO_2 eq	4.38E-03	4.38E-03	1.00
Eutrophication	kg PO_4^{3-} eq	6.14E-03	6.47E-03	0.95
Global warming 100a	kg CO_2 eq	1.64	-8.83E-01	-1.85
Ozone layer depletion steady state	kg CFC-11 eq	1.34E-08	1.38E-08	0.98
Human toxicity infinite	kg 1,4-DB eq	4.82E-01	4.46E-01	1.08
Fresh water aquatic ecotox. infinite	kg 1,4-DB eq	1.11E-02	2.12E-03	5.22
Marine aquatic ecotoxicity infinite	kg 1,4-DB eq	1.36E+01	6.63E+01	0.21

SimaPro: CML 2001 (version 2.05 from Nov 2009). GaBi: CML 2001: (Nov 2009). Acronyms: *S* SimaPro, *G* GaBi.

5.3 Comparison of aggregated impact potentials obtained for the OBM

In order to judge potential consequences of the observed differences when the results are used for decision support, the combined effects of differences in inventory and impact assessment are studied for the OBM object. The weighted and summed impact assessment results are sometimes used for decision support and they are compared for the OBM object in Table 6 using the EDIP 2003 methodology. From Table 6 it can be observed that there is a ratio of 12.2 between the results from SimaPro and GaBi. This ratio is strongly influenced by the Global warming and Photochemical ozone formation impact values which were shown in Table 2 to deviate strongly between SimaPro and GaBi. If these two impact categories were eliminated, the ratio between the aggregated results for the rest of the non-toxic impact categories would be 0.92.

Table 6. Aggregated impact potentials for the non-toxic impact categories obtained by summing the weighted results for the OBM object (Pt is targeted person equivalents)

Impact category	Unit	SimaPro	GaBi	Ratio S/G
Total	Pt	3.08E-06	3.75E-05	0.082
Global warming 100a	Pt	-1.96E-06	2.73E-05	
Ozone depletion	Pt	3.68E-07	3.42E-07	
Ozone formation (Vegetation)	Pt	-3.63E-06	-2.87E-06	
Ozone formation (Human)	Pt	-4.41E-06	-8.98E-08	
Acidification	Pt	2.43E-06	2.37E-06	
Terrestrial eutrophication	Pt	1.03E-05	1.05E-05	

5.4 Rechecking newer versions of GaBi and SimaPro

In order to check whether the main differences found in this paper had been eliminated in newer software versions, we updated Simapro (to version 7.3.2 Faculty version) and GaBi (to version 4.4.135.1). Here we found that the handling of biogenic carbon in all the compared impact assessment methods has not changed in the newer versions. Furthermore, we found that the difference in CFs relating to Photochemical ozone formation still differed among the software, as found in Table 3. Finally, the handling of the normalization and weighting in Eco-Indicator 99 had not changed either. Thus, we found no significant changes in these versions that would lead to adjusting the results in this paper. An even later version of GaBi (version 5) was released in November 2011, however at present (February 2012) we do not have access to this version of GaBi.

6 Conclusion

The goal of this paper was to assess if it can make a difference for the results of an LCA whether SimaPro or GaBi is used for modeling the product system and doing the impact assessment. The results have shown many differences both at the inventory level and in the impact assessment. Some of these differences are so large that it could influence the conclusions drawn from the study. There are potentially three main reasons that can cause differences in the results:

a. Differences in modeling assumptions and procedures of how to incorporate models into the software, such as numbers of emission compartments, way to model avoided production etc.
b. Differences in how the LCA practitioners (in this case the authors of this paper) handle the modeling in “a” above and implement the exact same data into the software
c. Differences in the applied databases (inventory and impact assessment)

We have done our utmost to eliminate the causes “a” and “b” by modeling the exact same systems, taking the modeling differences in the two software into consideration, and taking extreme care to avoid introduction of any differences in this regard. From the analysis it thus seems that the main reasons for the observed differences are to be found in c: differences in the applied databases. For the differences in the applied databases we have observed that these differences are found at; the unit process level, at the interface between the inventory and the characterization models, and at the characterized-, normalized-, and weighted level. The EcoInvent unit process on hydrochloric acid obtained from SimaPro and GaBi resulted in a maximum ratio, observed in this analysis, of a factor 1380 for CFC-11 to air. For the OBM object, based on EDIP 2003, at the characterized-, normalized-, and weighted level the maximum ratios were 102, 102 and 91.6 for Photochemical ozone formation (Human). For the aggregated EDIP2003 impact potentials obtained for the OBM object, the difference between SimaPro and GaBi was observed to be a ratio 12.

7 Recommendations

Some errors were identified in the implementation of the EDIP2003 methodology in one of the software but which one of the two analyzed software is correct in the total results is not possible to tell since falsification (or validation) of the performed LCAs are not possible in practice. Therefore it is highly problematic when two of the most widely used software gives such different results at all levels. It is clearly in the interest of both software developers and LCA practitioners that the observed differences are addressed in the future update of these software tools and more broadly in the development of LCA decision support tools in general. To identify and eliminate errors and unwanted differences in results between the different software, some sort of comparison-based validation should be performed systematically involving all the major LCA software producers, e.g. in the form of standardized ring tests as known from the validation of chemical analytical laboratories. The alternative is a loss of credibility that may jeopardize the professional use of LCA as decision support tool in the future.

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SUPPORTING INFORMATION

Title:	**Does it matter which LCA tool you choose?**
	- comparative assessment of SimaPro and GaBi on a biodiesel case study
Journal name:	**The International Journal of Life Cycle Assessment**

Ivan T. Herrmann*, Andreas Jørgensen, Morten Birkved, and Michael Z. Hauschild

Institute of Management Engineering, Section of Quantitative Sustainability Assessment, Technical University of Denmark, Produktionstorvet, building 426, DK-2800, Kgs. Lyngby, Denmark

*Corresponding author: ivan.t.h.business@gmail.com

P: +45 22756975

F: +45 45933435

S1) Comparison of inventories from SimaPro and GaBi obtained from identical product system models

S2) OBM (excluding HCL)

S3) Full inventory comparison of the AUP hydrochloric acid process obtained from EcoInvent.

S4) Comparison of inventories from SimaPro and GaBi obtained from identical unit process – SBF (1)

S5) Comparison of inventories from SimaPro and GaBi obtained from identical unit process – SBF (2)

S6) Comparison of characterized, normalized and weighted impact potentials for the SBF using the LCIA method Ecoindicator 99 – Egalitarian approach

Table S1 shows for each impact category the ratios between those three elementary flows from the SimaPro and GaBi inventories that have identical names in the two tools and/or have large characterization factors, as described in the method section. Table S1 is split into three main rows:

Environmental impacts, Resource Consumption (RC), and Toxicological impacts. All output values are in kg or MJ (according to the functional unit). Furthermore, Table S1 is split into two main columns: Name of substance and specific compartment (e.g. air or soil). Table S1 shows considerable differences between the GaBi and SimaPro.

Table S1. Comparison of inventory flows for 1 MJ biodiesel passenger car transportation based on the OBM object.

IC	IP	Emission	Comp.	Comp. specific emissions		
				S (kg)	G (kg)	Ratio (S/G)
EI	AP	Nitrogen oxides	air	2.56E-04	2.56E-04	1.00
		Sulfur dioxide	air	-1.75E-07	-2.09E-07	0.84
		Hydrogen chloride	air	-2.02E-07	-2.05E-07	0.98
	GWP	Carbon dioxide	air	1.28E-01	1.28E-01	1.00
		Carbon monoxide	air	9.70E-05	9.93E-05	0.98
		Methane	air	-2.42E-04	-2.42E-04	1.00
	NEP	Phosphorus	water	-1.41E-05	-1.41E-05	1.00
		Nitrate	water	4.65E-03	4.65E-03	1.00
		Nitrous oxide (N2O)	air	7.92E-05	7.92E-05	1.00
	ODP	CFC-11	air	3.02E-15	2.88E-15	1.05
		Carbon tetrachloride	air	2.87E-10	2.86E-10	1.00
		CFC-114	air	3.20E-12	2.52E-12	1.27
	POP (high)	Tetrafluoromethane	air	-6.82E-12	-5.09E-11	1.05
		Butane	air	1.23E-07	1.23E-07	1.00
		Benzene	air	-7.50E-06	-7.50E-06	1.00
	POP (low)	CFC-113	air	2.85E-13	2.71E-13	1.05
		Butene	air	1.63E-09	1.63E-09	1.00
		Phenol	air	-1.06E-07	-1.06E-07	1.00
RC	-	Nitrogen in air/atmosphere	-	3.33E-04	-3.33E-04	-1.00
		Crude Oil (in ground)	-	1.20E-03	1.21E-03	1.00
		Gravel/aggregate	-	3.46E-03	3.45E-03	1.00
TI	ES (chronic)	2,4-D	soil	-1.18E-05	-1.18E-05	1.00
		Cadmium	soil	-2.28E-08	-2.28E-08	1.00
		Clomazone	soil	1.96E-06	1.96E-06	1.00
	EW (acute)	Alpha-cypermethrin	water	1.80E-08	1.80E-08	1.00
		Azoxystrobin	water	3.18E-09	3.18E-09	1.00
		Lead/Lead(II)	water	-1.33E-09	-1.18E-09	1.13
	EW (chronic)	Clopyralid	water	1.11E-08	1.11E-08	1.00
		Tebuconazole	water	6.14E-08	6.14E-08	1.00
		Mercury/Mercury(II)	water	-1.21E-09	-1.22E-09	1.00

HT(air)	2,3,7,8 - TCDD	air	2.61E-15	2.59E-14	0.10
	Hexane	air	-8.58E-05	-8.58E-05	1.00
	Antimony	air	1.67E-10	1.60E-10	1.04
HT(soil)	Napropamide	soil	2.54E-08	2.54E-08	1.00
	Zinc/Zinc(II)	soil	1.59E-06	1.59E-06	1.00
	Nickel/Nickel (II)	soil	1.39E-07	1.39E-07	1.00
HT(water)	Cumene	water	1.11E-09	1.11E-09	0.99
	Thallium	water	-3.50E-12	-4.75E-12	0.74
	Copper/Copper (II)	water	2.59E-09	4.51E-09	0.57

Acronyms: *S* SimaPro, *G* GaBi, *IC* Impact Category, *IP* Impact Potential, *EI* Environmental Impacts, *RC* Ressource Consumptions, *TI* Toxicological Impacts, *AP* Acidification Potential, *Comp.* Compartment, *ES(chronic)* Ecotoxicity Soil chronic, *EW(acute)* Ecotoxicity water acute, *EW(chronic)* Ecotoxicity water chronic, *GWP* Global Warming Potential (GWP 100 years), *HT(air)* Human Toxicity air, *HT(soil)* Human toxicity soil, *HT(water)* Human Toxicity water, *IP* Impact Potential, *NEP* Nutrient Enrichment Potential, *ODP* Ozone Depletion Potential, *POP(high)* Photochemical Ozone formation Potential (high NOx), *POP(low)* Photochemical Ozone formation Potential (low NOx), *RC* Resource Consumptions, *Soil* Agricultural soil and industrial soil, *Water* fresh water and seawater.

The output values shown in Table S2+S3 have been selected applying the criteria described in the method section in main manuscript. Table S2+S3 are split into three main rows: Environmental Impacts, Resource Consumption (RC), and Toxicological Impacts. All output values are in kg or MJ (according to the functional unit). Furthermore, Table S2+S3 are split into three main columns: Name of emissions, compartment with specific emission, and emissions to all compartments. The reason for presenting both “compartment with specific emission” and “emissions to all compartments” columns is to check that the observed differences in the compartment with specific emission are not due to a *swop* between the specific compartments. If the “emission to all compartments” reveals same difference as the specific compartments then we assume that there is no such swop between the specific emissions compartments.

Table S2. OBM (excluding HCL)

IC	IP	Emission	Comp.	Comp. specific emissions			Comp.	Emissions to all comp. (excluding raw materials)		
				S (kg)	G (kg)	Ratio (S/G)		S (kg)	G (kg)	Ratio (S/G)
EI	AP	Nitrogen oxides	air	1.87E-04	1.87E-04	1.00	all	1.87E-04	1.87E-04	1.00
		Sulfur dioxide	air	-2.92E-05	-2.92E-05	1.00	all	-2.92E-05	-2.92E-05	1.00
		Hydrogen chloride	air	-5.01E-07	-5.01E-07	1.00	all	-5.01E-07	-5.01E-07	1.00
	GWP	Carbon dioxide	air	8.80E-02	8.80E-02	1.00	all	8.80E-02	8.80E-02	1.00
		Carbon monoxide	air	-1.39E-03	-1.39E-03	1.00	all	-1.39E-03	-1.39E-03	1.00
		Methane	air	-3.54E-04	-3.54E-04	1.00	all	-3.54E-04	-3.54E-04	1.00
	NEP	Phosphorus	water	-2.46E-05	-2.46E-05	1.00	all	-2.46E-05	-2.46E-05	1.00
		Nitrate	water	3.48E-03	3.48E-03	1.00	all	3.48E-03	3.48E-03	1.00
		Nitrous oxide (N2O)	air	4.33E-05	4.33E-05	1.00	all	4.33E-05	4.33E-05	1.00
	ODP	CFC-11	air	2.05E-15	2.05E-15	1.00	all	2.05E-15	2.05E-15	1.00
		Carbon tetrachloride	air	4.06E-12	4.06E-12	1.00	all	4.06E-12	4.06E-12	1.00
		CFC-114	air	-1.16E-11	-1.16E-11	1.00	all	-1.16E-11	-1.16E-11	1.00
	POP (high)	Tetrafluoromethane	air	-1.45E-09	-1.45E-09	1.00	all	-1.45E-09	-1.45E-09	1.00
		Butane	air	2.40E-08	2.40E-08	1.00	all	2.40E-08	2.40E-08	1.00
		Benzene	air	-1.33E-05	-1.33E-05	1.00	all	-1.33E-05	-1.33E-05	1.00
	POP (low)	CFC-113	air	1.94E-13	1.94E-13	1.00	all	1.94E-13	1.94E-13	1.00
		Butene	air	1.26E-10	1.26E-10	1.00	all	1.43E-10	1.44E-10	1.00
		Phenol	air	-1.87E-07	-1.87E-07	1.00	all	-1.56E-07	-1.56E-07	1.00
RC	-	Nitrogen in air/atmosphere	-	3.33E-04	-3.33E-04	-1.00		-	-	-
		Crude Oil (in ground)	-	8.04E-05	8.05E-05	1.00		-	-	-
		Gravel/aggregate	-	1.30E-03	1.30E-03	1.00		-	-	-
TI	ES (chronic)	2,4-D	soil	-2.07E-05	-2.07E-05	1.00	all	-2.07E-05	-2.07E-05	1.00
		Cadmium	soil	-3.50E-08	-3.50E-08	1.00	all	-5.09E-08	-5.09E-08	1.00
		Clomazone	soil	1.96E-06	1.96E-06	1.00	all	1.96E-06	1.96E-06	1.00
	EW (acute)	Alpha-cypermethrin	water	1.80E-08	1.80E-08	1.00	all	4.71E-07	4.72E-07	1.00
		Azoxystrobin	water	3.18E-09	3.18E-09	1.00	all	1.26E-06	1.26E-06	1.00
		Lead/Lead(II)	water	-1.10E-08	-1.10E-08	1.00	all	-1.50E-07	-1.50E-07	1.00
	EW (chronic)	Clopyralid	water	1.11E-08	1.11E-08	1.00	all	1.62E-06	1.62E-06	1.00
		Tebuconazole	water	6.14E-08	6.14E-08	1.00	all	2.58E-06	2.58E-06	1.00
		Mercury/Mercury(II)	water	-2.65E-09	-2.65E-09	1.00	all	-2.58E-09	-2.58E-09	1.00
	HT(air)	2,3,7,8-TCDD	air	2.22E-16	7.97E-16	0.28	all	2.22E-16	7.97E-16	0.28
		Hexane	air	-1.51E-04	-1.51E-04	1.00	all	-1.51E-04	-1.51E-04	1.00
		Antimony	air	3.96E-11	3.96E-11	1.00	all	2.10E-09	2.10E-09	1.00
	HT(soil)	Napropamide	soil	2.45E-08	2.45E-08	1.00	all	2.45E-08	2.45E-08	1.00
		Zinc/Zinc(II)	soil	2.63E-06	2.63E-06	1.00	all	2.76E-06	2.76E-06	1.00
		Nickel/Nickel (II)	soil	2.49E-07	2.49E-07	1.00	all	2.63E-07	2.63E-07	1.00
	HT(water)	Cumene	water	1.14E-10	1.15E-10	1.00	all	1.62E-10	1.62E-10	1.00
		Thallium	water	-4.57E-11	-4.58E-11	1.00	all	-6.40E-11	-6.40E-11	1.00
		Copper/Copper (II)	water	-1.82E-08	-1.82E-08	1.00	all	1.10E-06	1.10E-06	1.00

Acronyms: *S* SimaPro, *G* GaBi, *IC* Impact Category, *IP* Impact Potential, *EI* Environmental Impacts, *RC* Ressource Consumptions, *TI* Toxicological Impacts, *AP* Acidification Potential, *Comp.* Compartment, *ES(chronic)* Ecotoxicity Soil chronic, *EW(acute)* Ecotoxicity water acute, *EW(chronic)* Ecotoxicity water chronic, *GWP* Global Warming Potential (GWP 100 years), *HT(air)* Human Toxicity air, *HT(soil)* Human toxicity soil, *HT(water)* Human Toxicity water, *IP* Impact Potential, *NEP* Nutrient Enrichment Potential, *ODP* Ozone Depletion Potential, *POP(high)* Photochemical Ozone formation Potential (high NOx), *POP(low)* Photochemical Ozone formation Potential (low NOx), *RC* Resource Consumptions, *Soil* Agricultural soil and industrial soil, *Water* fresh water and seawater.

Table S3. Inventory comparison of the AUP hydrochloric acid process obtained from EcoInvent.

IC	IP	Emission	Comp.	Comp. specific emissions			Comp.	Emissions to all comp. (excluding raw materials)		
				S (kg)	G (kg)	Ratio (S/G)		S (kg)	G (kg)	Ratio (S/G)
EI	AP	Nitrogen oxides	air	1.66E-03	1.62E-03	1.02	all	1.66E-03	1.62E-03	1.02
		Sulfur dioxide	air	3.03E-03	2.90E-03	1.05	all	3.03E-03	2.90E-03	1.05
		Hydrogen chloride	air	5.09E-05	3.75E-05	1.36	all	5.09E-05	3.75E-05	1.36
	GWP	Carbon dioxide	air	8.65E-01	7.36E-01	1.18	all	8.65E-01	7.36E-01	1.18
		Carbon monoxide	air	1.40E-03	6.26E-04	2.23	all	1.40E-03	6.26E-04	2.23
		Methane	air	1.70E-03	9.77E-04	1.73	all	1.70E-03	9.77E-04	1.73
	NEP	Phosphorus	water	4.63E-07	3.07E-07	1.51	all	8.13E-07	5.22E-07	1.56
		Nitrate	water	2.77E-04	2.76E-04	1.00	all	2.77E-04	2.76E-04	1.00
		Nitrous oxide (N2O)	air	2.37E-05	2.39E-05	0.99	all	2.37E-05	2.39E-05	0.99
	ODP	CFC-11	air	5.88E-13	4.26E-16	1380.38	all	5.88E-13	4.26E-16	1380.38
		Carbon tetrachloride	air	1.10E-06	1.10E-06	1.00	all	1.10E-06	1.10E-06	1.00
		CFC-114	air	6.92E-09	4.34E-09	1.59	all	6.92E-09	4.34E-09	1.59
	POP (high)	Tetrafluoromethane	air	2.12E-07	3.73E-08	5.68	all	2.12E-07	3.73E-08	5.68
		Butane	air	5.96E-06	5.45E-06	1.09	all	5.96E-06	5.45E-06	1.09
		Benzene	air	3.64E-06	4.19E-06	0.87	all	4.00E-06	4.52E-06	0.89
	POP (low)	CFC-113	air	5.45E-11	0.00E+00	na.	all	5.45E-11	0.00E+00	na.
		Butene	air	6.56E-08	7.08E-08	0.93	all	6.56E-08	7.08E-08	0.93
		Phenol	air	5.24E-08	6.75E-09	7.77	all	3.67E-07	4.38E-07	0.84
RC	-	Nitrogen in air/atmosphere	-	0.00E+00	0.00E+00	na.	all	0.00E+00	0.00E+00	na.
		Crude Oil (in ground)	-	5.89E-02	6.04E-02	0.98	all	5.89E-02	6.04E-02	0.975149
		Gravel/aggregate	-	1.09E-01	7.81E-02	1.40	all	1.09E-01	7.81E-02	1.40128
TI	ES (chronic)	2,4-D	soil	3.14E-11	0.00E+00	na.	all	3.14E-11	0.00E+00	na.
		Cadmium	soil	1.09E-09	1.55E-09	0.70	all	1.93E-07	2.36E-07	0.82
		Clomazone	soil	0.00E+00	0.00E+00	na.	all	0.00E+00	0.00E+00	na.
	EW (acute)	Alpha-cypermethrin	water	0.00E+00	0.00E+00	na.	all	0.00E+00	0.00E+00	na.
		Azoxystrobin	water	0.00E+00	0.00E+00	na.	all	0.00E+00	0.00E+00	na.
		Lead/Lead(II)	water	9.22E-07	1.43E-06	0.64	all	2.05E-06	2.09E-06	0.98
	EW (chronic)	Clopyralid	water	0.00E+00	0.00E+00	na.	all	0.00E+00	0.00E+00	na.
		Tebuconazole	water	2.77E-05	0.00E+00	na.	all	2.77E-05	0.00E+00	na.
		Mercury/Mercury(II)	water	6.37E-08	5.99E-08	1.06	all	4.35E-07	3.74E-07	1.16
	HT(air)	2,3,7,8 - TCDD	air	4.29E-13	9.03E-11	0.00	all	4.29E-13	9.03E-11	0.00
		Hexane	air	3.19E-06	2.75E-08	115.78	all	3.19E-06	2.75E-08	115.78
		Antimony	air	4.39E-08	1.59E-08	2.77	all	1.01E-06	8.82E-07	1.15
	HT(soil)	Napropamide	soil	5.95E-12	3.66E-12	1.63	all	5.95E-12	3.66E-12	1.63
		Zinc/Zinc(II)	soil	3.46E-07	5.53E-07	0.63	all	1.25E-04	2.69E-04	0.46
		Nickel/Nickel (II)	soil	1.12E-08	4.73E-08	0.24	all	1.59E-05	1.24E-05	1.28
	HT(water)	Cumene	water	1.15E-07	2.07E-07	0.55	all	1.62E-07	2.07E-07	0.79
		Thallium	water	1.48E-08	1.00E-08	1.47	all	1.51E-08	1.03E-08	1.47
		Copper/Copper (II)	water	2.95E-06	1.06E-05	0.28	all	4.50E-06	1.16E-05	0.39

Table S4. Comparison of selected inventory flows from SimaPro and GaBi for the unit process – SBF (1)

IC	IP	Emission	Comp.	Comp. specific emissions			Comp.	Emissions to all comp. (excluding raw materials)		
				S (kg)	G (kg)	Ratio (S/G)		S (kg)	G (kg)	Ratio (S/G)
EI	AP	Nitrogen oxides	air	1.91E-03	1.91E-03	1.00	all	1.91E-03	1.91E-03	1.00
		Sulfur dioxide	air	7.62E-04	7.62E-04	1.00	all	7.62E-04	7.62E-04	1.00
		Hydrogen chloride	air	2.30E-06	2.30E-06	1.00	all	2.30E-06	2.30E-06	1.00
	GWP	Carbon dioxide	air	1.13E+00	1.13E+00	1.00	all	1.13E+00	1.13E+00	1.00
		Carbon monoxide	air	4.91E-02	4.91E-02	1.00	all	4.91E-02	4.91E-02	1.00
		Methane	air	3.37E-03	3.37E-03	1.00	all	3.37E-03	3.37E-03	1.00
	NEP	Phosphorus	water	3.46E-04	3.46E-04	1.00	all	3.46E-04	3.46E-04	1.00
		Nitrate	water	3.88E-02	3.88E-02	1.00	all	3.88E-02	3.88E-02	1.00
		Nitrous oxide (N2O)	air	1.91E-03	1.91E-03	1.00	all	1.91E-03	1.91E-03	1.00
	ODP	CFC-11	air	2.29E-14	2.29E-14	1.00	all	2.29E-14	2.29E-14	1.00
		Carbon tetrachloride	air	1.10E-10	1.10E-10	1.00	all	1.10E-10	1.10E-10	1.00
		CFC-114	air	3.02E-10	3.02E-10	1.00	all	3.02E-10	3.02E-10	1.00
	POP (high)	Tetrafluoromethane	air	4.08E-08	4.08E-08	1.00	all	4.08E-08	4.08E-08	1.00
		Butane	air	1.51E-06	1.51E-06	1.00	all	1.51E-06	1.51E-06	1.00
		Benzene	air	1.91E-04	1.91E-04	1.00	all	1.91E-04	1.91E-04	1.00
	POP (low)	CFC-113	air	2.13E-12	2.13E-12	1.00	all	2.13E-12	2.13E-12	1.00
		Butene	air	3.01E-08	3.01E-08	1.00	all	3.02E-08	3.02E-08	1.00
		Phenol	air	2.67E-06	2.67E-06	1.00	all	2.79E-06	2.79E-06	1.00
RC	-	Nitrogen in air/atmosphere	-	0.00E+00	0.00E+00	-		-	-	-
		Crude Oil (in ground)	-	2.26E-02	2.26E-02	1.00		-	-	-
		Gravel/aggregate	-	3.88E-02	3.88E-02	1.00		-	-	-
TI	ES (chronic)	2,4-D	soil	2.95E-04	2.95E-04	1.00	all	2.95E-04	2.95E-04	1.00
		Cadmium	soil	4.05E-07	4.05E-07	1.00	all	6.42E-07	6.42E-07	1.00
		Clomazone	soil	0.00E+00	0.00E+00	-	all	-	-	-
	EW (acute)	Alpha-cypermethrin	water	0.00E+00	0.00E+00	-		-	-	-
		Azoxystrobin	water	0.00E+00	0.00E+00	-		-	-	-
		Lead/Lead(II)	water	2.93E-07	2.93E-07	1.00	all	2.52E-06	2.52E-06	1.00
	EW (chronic)	Clopyralid	water	0.00E+00	0.00E+00	-		-	-	-
		Tebuconazole	water	0.00E+00	0.00E+00	-		-	-	-
		Mercury/Mercury(II)	water	4.66E-08	4.66E-08	1.00	all	5.21E-08	5.21E-08	1.00
	HT(air)	2,3,7,8 - TCDD	air	5.86E-14	5.86E-14	1.00	all	5.86E-14	5.86E-14	1.00
		Hexane	air	7.70E-07	7.70E-07	1.00	all	7.70E-07	7.70E-07	1.00
		Antimony	air	3.20E-09	3.20E-09	1.00	all	4.13E-08	4.13E-08	1.00
	HT(soil)	Napropamide	soil	3.01E-08	3.01E-08	1.00	all	3.01E-08	3.01E-08	1.00
		Zinc/Zinc(II)	soil	-3.45E-05	-3.45E-05	1.00	all	-3.23E-05	-3.23E-05	1.00
		Nickel/Nickel (II)	soil	-3.66E-06	-3.66E-06	1.00	all	-1.57E-06	-1.57E-06	1.00
	HT(water)	Cumene	water	2.17E-08	2.17E-08	1.00	all	3.08E-08	3.08E-08	1.00
		Thallium	water	5.00E-10	5.00E-10	1.00	all	5.47E-10	5.47E-10	1.00
		Copper/Copper (II)	water	6.14E-07	6.14E-07	1.00	all	-1.16E-05	-1.16E-05	1.00

In Table S5 the summed in- and output flows for: mass (kg); energy (MJ); radioactivity (Bq); and area (m^2) are presented for the SBF object. The column "S/G" presents the ratios between SimaPro and GaBi which are based on the balance columns for SimaPro respectively GaBi. We accept the results to be categorized as "no difference" even though a small difference is observed.

Table S5. Comparison of inventories from SimaPro and GaBi obtained from identical unit process – SBF (2). Flow balance showing an acceptable level of similarity between the two inventories for SBF based on total mass-, energy-, radioactivity-, and areal balance.

	SimaPro			GaBi			S/G
	Input	Output	Balance	Input	Output	Balance	Ratio
Mass/[kg]	1.621E+00	1.327E+00	-2.942E-01	1.621E+00	1.327E+00	-2.946E-01	0.999
Energy/[MJ]	2.994E+01	1.690E+00	-2.825E+01	2.994E+01	1.690E+00	-2.825E+01	1.000
Radiation/[Bq]	0.000E+00	1.904E+04	1.904E+04	0.000E+00	1.910E+04	1.910E+04	0.997
Area/[m^2]	8.452E+00	0.000E+00	-8.452E+00	8.452E+00	0.000E+00	-8.452E+00	1.000

Table S6. Comparison of characterized, normalized and weighted impact potentials for the SBF using the LCIA method Ecoindicator 99 – Egalitarian approach.

	Characterized				Normalized			Weighted		
Impact category	Units	S	G	Ratio	S (PE)	G (PE)	Ratio	S (Pt)	G (Pt)	Ratio
Carcinogens	DALY	9.76E-07	8.91E-07	1.10	6.32E-05	4.46E-04	0.14	1.89E-02	1.72E-02	1.10
Respiratory organics	DALY	6.21E-09	6.36E-09	0.98	4.02E-07	9.30E-05	0.00	1.21E-04	1.23E-04	0.98
Respiratory inorganics	DALY	3.60E-06	3.61E-06	1.00	2.33E-04	3.34E-04	0.70	6.98E-02	6.99E-02	1.00
Climate change	DALY	3.50E-07	3.56E-08	9.84	2.27E-05	1.49E-05	1.52	6.80E-03	6.88E-04	9.87
Radiation	DALY	4.61E-10	3.19E-09	0.14	2.98E-08	1.19E-04	0.00	8.95E-06	6.16E-05	0.15
Ozone layer	DALY	1.41E-11	1.41E-11	1.00	9.14E-10	6.45E-08	0.01	2.74E-07	2.73E-07	1.00
Ecotoxicity	PDF.m2.yr	3.81E-03*	3.66E-03	1.04	7.43E-07	4.51E-06	0.16	3.72E-04	3.56E-04	1.04
Acidification/ Eutrophication	PDF.m2.yr	3.62E-02	3.61E-02	1.00	7.06E-06	9.62E-05	0.07	3.53E-03	3.51E-03	1.00
Land use	PDF.m2.yr	7.74E+00	2.39E+00	3.24	1.51E-03	6.06E-04	2.49	7.55E-01	2.33E-01	3.24
Minerals	MJ surplus	1.00E-02	8.45E-03	1.18	1.68E-06	5.71E-05	0.03	3.36E-04	2.85E-04	1.18
Fossil fuels	MJ surplus	1.22E-01	1.27E-01	0.96	2.06E-05	2.19E-05	0.94	4.11E-03	4.28E-03	0.96
Land conversion	[PDF.m2]	NA	5.06E+00	NA	NA	1.28E-03	NA	NA	0.49E-03	NA

*Results from SimaPro in PAF.m^2.yr converted to PDF.m^2.yr by multiplication with 0.1 PDF/PAF according to Larsen and Hauschild (2007).

Appendix D: Enabling optimization in LCA: from the ad hoc to the Structural LCA approach

- Based on a biodiesel well-to-wheel case study

Authors: Ivan T. Herrmann, Martin Lundberg-Jensen, Andreas Jørgensen, Thomas Stidsen, Henrik Spliid, and Michael Hauschild

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Title: **Enabling optimization in LCA: from "Ad hoc" to "Structural" LCA approach**

- **based on a biodiesel well-to-wheel case study**

Authors:

Ivan T. Herrmann[a,*], Martin Lundberg-Jensen[b], Andreas Jørgensen[a], Thomas Stidsen[b], Henrik Spliid[c], and Michael Hauschild[a]

*Corresponding author: ivan.t.h.business@gmail.com; P: +45 22756975; F: +45 45933435

[a]Division of Quantitative Sustainability Assessment, Department of Management Engineering, Technical University of Denmark, Produktionstorvet, Building 424, DK-2800, Kgs. Lyngby, Denmark

[b]Division of Management Science, Department of Management Engineering, Technical University of Denmark, Produktionstorvet, Building 424, DK-2800, Kgs. Lyngby, Denmark

[c]Department of Informatics and Mathematical Modeling, Technical University of Denmark, Building 305, DK-2800, Kgs. Lyngby, Denmark

1 Abstract

Background, aim, and scope.

Applied life cycle assessment (LCA) studies often lead to comparison of rather few alternatives, we call this the "*Ad hoc* LCA approach". This can seem surprising since applied LCAs normally cover countless options for variations and derived potentials for improvements in a product life cycle. In this paper we will suggest an alternative approach to the Ad hoc approach, which more systematically addresses the many possible variations to identify the most promising. We call it the "*Structural* LCA approach". The goal of this paper is 1) to provide basic guidelines for the Structural approach including an easy expansion of the LCA space; 2) to show that the Structural LCA approach can be used for different types of optimization in LCA; and 3) to improve transparency of the LCA work.

Methods.

The Structural approach is based on the methodology "Design of Experiments" (DOE) (Montgomery 2005). Through a biodiesel well-to-wheel (WTW) study we demonstrate a generic approach of applying explanatory variables and corresponding impact categories within the LCA methodology. Furthermore, using the Structural approach enables two different possibilities for optimization; 1) single-objective optimization (SO) based on response surface methodology (Montgomery 2005), and 2) multi-objective optimization (MO) by the Hyper-volume Estimation Taboo Search (HETS) method. HETS enables MO for more than 2 or 3 objectives.

Results and discussion.

Using single-objective optimization (SO), the explanatory variable "use of residual straw from fields" is, by far, the explanatory variable that can contribute with the highest decrease of Climate change potential. For the Respiratory inorganics impact category the most influencing explanatory variable is found to be the use of different Alcohol types (bioethanol or petrochemical methanol) in the biodiesel production. Using multi-objective optimization (MO) we found the Pareto front based on five different life cycle pathways which are non-dominated solutions out of 66 different analyzed

solutions. Given that there is a fixed amount of resources available for the LCA practitioner it becomes a prioritizing problem whether to apply the Structural LCA approach or not. If the decision maker only has power to change a single explanatory variable it might not be beneficial to apply the Structural LCA approach. However, if the decision maker (such as decision makers at the societal level) has power to change more explanatory variables then the Structural LCA approach seems beneficial for quantifying and comparing the potentials for environmental improvement between the different explanatory variables in an LCA system and identifying the overall most promising product system configurations among the chosen PWs.

Conclusion and recommendations.

The implementation of the Structural LCA approach and the derived use of SO and MO has been successfully achieved and demonstrated in the present paper. In addition, it is demonstrated that the structural LCA approach can lead to more transparent LCAs since the potentially most important explanatory variables which are used to model the LCAs are explicitly presented through the Structural LCA approach. The suggested Structural approach is a new approach to LCA and it seems to be a promising approach for searching or screening product systems for environmental optimization potentials. In the presented case the design has been a rather simple full factorial design. More complicated problems or designs, such as fractional designs, nested designs, split plot designs, and/or unbalanced data in the context of LCA could be investigated further using the Structural approach.

Keywords: LCA, optimization, structural approach, design of experiments, rapeseed biodiesel.

2 Introduction

Life Cycle Assessment (LCA) offers a quantitative approach to assess environmental impacts from products, technologies and services (Wenzel, Hauschild & Alting 1997; Finnveden et al. 2009; EC-JRC 2010). LCA's are conducted by LCA practitioners to support decision for making the best possible choice for the environment.

Product systems can include many processes and in many cases variations of these processes are possible which can result in a very large number of possible combinations – or alternative life cycle pathways (PW). Each new PW we regard as an additional solution to the LCA *space*. In applied LCAs, the potential variations are most often considered in a not systematic *Ad hoc* manner, where only a very limited number of variations are considered leading to the risk that more optimal alternatives are overlooked, we call this the "Ad hoc LCA approach". In this article we present a more systematic approach to the development of the alternatives to investigate in the LCA which we will call the "*Structural* LCA approach". Here it becomes possible to create a much larger LCA space compared to the Ad hoc LCA approach and in addition it opens new options for analyzing and investigating the LCA space with focus on optimization. In the present paper we apply "Design of Experiments" (DOE) methodology based on Montgomery (2005). Since many LCA practitioners use software tools like SimaPro (pre.nl 2012) or GaBi (pe-international.com 2012) for the simulation of the product system, it should not require much more effort to expand the space of alternatives by varying different explanatory variables in the product system model and evaluate the outcome of these changes. The benefits of the Structural LCA approach, compared to the Ad hoc approach, can be four-fold:

1. Easy expansion of the space of alternatives by developing the structural *table*.
2. Based on Response surface methodology we can investigate which of the explanatory variables are the most influential for each response variable/impact category and hence derive optimal settings for each explanatory variable. This can be done by using statistical software tools (e.g. "R" (r-project.org 2012) which is freely available). We call this single-objective optimization (SO).
3. If the number of alternatives is sufficiently high then multi-objective optimization (MO) can be used as a non-subjective method to find the Pareto optimal alternatives[1] for the system and delimit the use of the often challenged value-based weighting step in the LCA.

[1] i.e. non dominated alternatives.

Furthermore the Hyper-volume Estimation Taboo Search (HETS) method that was developed for this project enables MO to be used for more than 2-3 objectives which is highly relevant for LCA that may operate with up to 15 different midpoint impact categories (Hauschild et al. 2012).

4. The reporting of the LCA can be more transparent if the explanatory variables are explicitly outlined with a distinction between explanatory variables that have been changed in the study and explanatory variables that have been kept constant ("ceteris paribus" approach).

The Structural LCA approach is explained and demonstrated through a WTW study of biodiesel developed within a 3-years LCA research program. Two Danish companies, Emmelev A/S (emmelev.dk 2012) (biodiesel refinery) and Novozymes A/S (novozymes.com 2012) (producer of industrial enzymes), have been partners with focus on optimization of the environmental performance of biodiesel in a WTW perspective.

Table 1. Terminology use and translation between LCA, statistics, and operations research including abbreviation for central concepts in this paper. Dash (-) indicates that there is no special terminology used in the given scientific field.

LCA	**Statistics/** (Montgomery 2005)	**Operations research**	**Abbreviation in this paper**
Life cycle assessment	-	-	LCA
-	-	Operations research	OR
The structural table	The design	-	-
-	Design of Experiments	-	DOE
Functional unit	Normalization	-	-
Pathway, scenario	Run	Solution	PW
LCA space	-	Space	-
Impact category	Response variable	Objective	-
Product system variables	Explanatory variables/ factors/treatments	-	-
Option or choice	Level	-	-
Process step	-	-	-
Well-to-wheel	-	-	WTW
-	-	Single-objective optimization	SO
-	-	Multi-objective optimization	MO
-	Dependency/interaction effect	-	-
-	Qualitative/discrete/categorical	-	-
-	Quantitative/continuous	-	-

3 Methods

First, we outline the Structural LCA approach, the SO approach, and the MO approach. Second we implement these methodologies in the WTW case study of biodiesel.

3.1 The Structural table

The Structural LCA approach is formulated through *the Structural table* as outlined in Table 2. Potentially we can look at e.g. 20 different explanatory variables, such as electricity supply and other fundamental technology choices, distance and means of transport, production equipment, additives, products that can be substituted (e.g. petrochemical fuels with biofuel), production location and so on. Each explanatory variable can be varied on a discrete or continuous scale. In this section we only consider discrete options, for example 20 explanatory variables each with four levels. Without any constraints this would be a problem of 4^{20} individual alternatives. In the context of LCA we will consider these alternatives as different PWs through the life cycle, representing (sometimes marginally) different product systems. Many of these PWs might not, *at present*, be technically possible or economically feasible. On the other hand if the environmental impact of some of these pathways turns out to be considerably low compared to a baseline scenario or business-as-usual scenario then investments for developing these pathways may be interesting to consider. The design of the Structural approach is not trivial and is highly dependent on the goal and scope of the LCA. For example, from a decision making point of view, it is relevant to consider how much influence the decision maker can exercise over the different explanatory variables. In an initial "screening" experiment it can be meaningful to operate with fewer levels than e.g. 4, as the number of PWs rapidly decreases, for example going from 4^{20} to 2^{20} is a reduction of PWs with a factor of ~ 1.05 million.

Table 2. The Structural table. Each pathway has a unique ID number ranging from 1-*l*. There are *n* explanatory variables. There can be *h* different levels for each explanatory variable. Dependency between the explanatory variables is investigated in the later optimization step. There are *m* different response variables. Abbreviation: *Obs*. Observation (or result).

PW	Explanatory variables					Response variables			
	X_1	X_2	…	X_n		Y_1	Y_2	…	Y_m
1	Level 1	Level 1		Level 1	=	Obs. 1	Obs. 1		Obs. 1
2	Level 2	Level 2		…	=	Obs. 2	Obs. 2		…
3	Level 3	…			=	Obs. 3	…		
4	…				=	…			
…					=				
l	Level *h*	…		…	=	…	…		…

3.1.1 Design of the Structural table and the application to LCA

An approach for the design of the Structural table can be to use an expert-panel to determine (Montgomery 2005):

a) The relevant explanatory variables
b) The relevant scale of the levels for each explanatory variable
c) The relevant response variables (if not all environmental impact categories)

For practical LCA application this might be an ongoing process during the LCA project. For illustration purpose Figure 1 shows a 2^4 factorial design with Electricity, Use of straw from field, choice of Alcohol and Transport distance of fuel as the four explanatory variables each with two levels: high (+) and low (-). For Alcohol "-" indicates the choice of Bioethanol and "+" indicates the choice of Petrochemical methanol. One approach in DOE is to select the starting point with all explanatory variables at the low level and then successively vary each variable over its range with the other variables held constant. When using LCA software tools like SimaPro or GaBi we would have to make a new run (simulation) for each PW with the new setting in our database (or model structure) and read off the new response values. When both the left side of Structural table (explanatory variables) and the right side (response variables) are populated with all the data, then several options for analyzing this table, based on SO and MO, becomes possible to support an optimized use of resources and reduced environmental impacts.

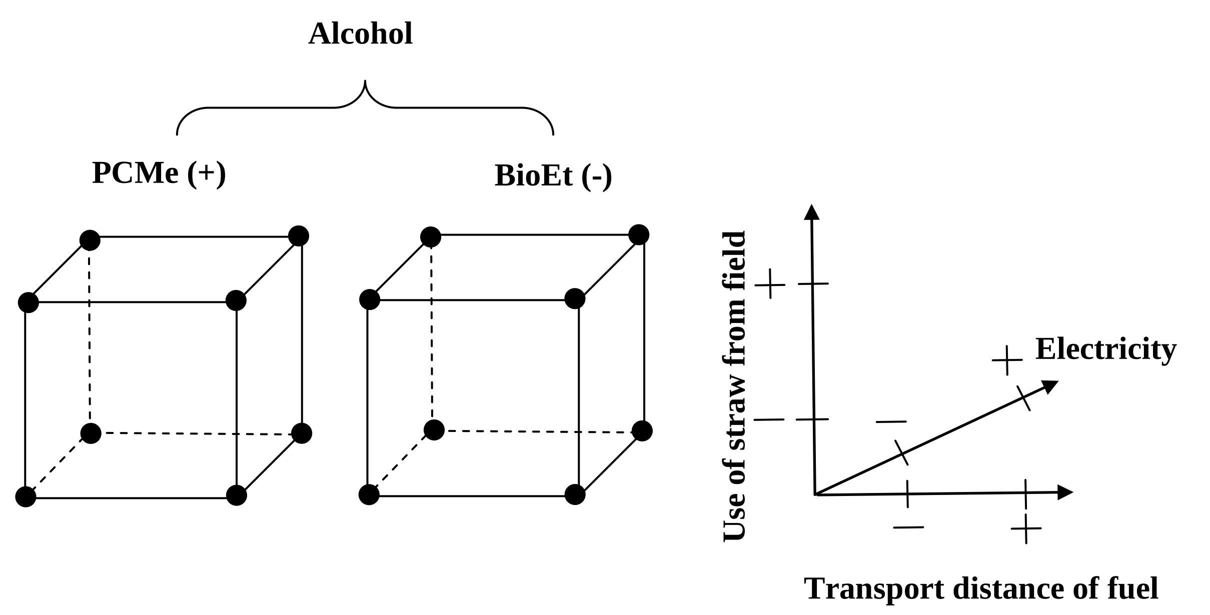

Figure 1. A full four-factor factorial design with two levels (2^4 design). Each corner in the two cubes (and the ends of the bracket) illustrates the high and low setting for run of the experiment. PCMe = petrochemical methanol; BioEt = Bioethanol.

In the design in Figure 1 there are four *main effects*, one from each explanatory variable. In designs with more than one explanatory variable ($2^{1<}$) there is a possibility for dependency between the different explanatory variables, this is called *interaction effects*. For small designs, say a 2^2 design, it is simple to compute, by hand, both the main effects and the interactions effects. Calculating the effect in a 2^1 design is done by subtracting the response variable value between the high and low level. However, to compute these effects by hand, rapidly becomes unrealistic and requires a statistical software tool as the number of explanatory variables. For a general procedure for calculating main effects and interaction effects we refer to Montgomery (2005).

3.2 Single-objective optimization

By using a statistical software tool, such as “R” (r-project.org 2012) which is freely available, we can translate the above Structural table into a statistical *effect* model (Equation 1). Based on this statistical model we can investigate and quantify which explanatory variables are the most influential on the specific impact category (response variable). In addition, if the explanatory variables are controllable for the decision maker, the stated model enables us to adjust the explanatory variables to achieve a reduction in the impact category. If the goal is to minimize the different environmental impacts then we can optimize according to these preferences. Equation 1 is the statistical effect model of a two-factor design with *a* levels for explanatory variable (or treatment) τ and *b* levels for the explanatory variable (or treatment) β.

Equation 1:

$$y_{ij} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \varepsilon_{ij} \begin{cases} i = 1,2,...,a \\ j = 1,2,...,b \end{cases}$$

y_{ij} is the observed response when explanatory variable or treatment τ is at the *i*th level (*i* = 1, 2,…, *a*) and explanatory variable β is at the *j*th level (*j* = 1,2,…, *b*), μ is a parameter common to all treatments called the *overall* mean (or the *intercept*), $(\tau\beta)_{ij}$ is the interaction effect between τ_i is and β_j, and the ε_{ij} is a random error component that incorporates all other sources of variability in the PW including measurement variability, variability arising from uncontrolled factors, the general background noise in the processes (such as variability over time, effects of environmental variables, and so forth). The interpretation of this model is that μ is a constant and the treatment effects τ_i, β_j, and the interaction effect $(\tau\beta)_{ij}$ represent deviations from the constant (μ) when the specific treatments are applied (Montgomery 2005). When simulating the effects on environmental impacts through the software tools SimaPro or GaBi we would not expect any random error effects $(\varepsilon)_{ij}$ to occur. Another way to investigate the potentials for optimization is to calculate the sum of squares (or least square estimates). The sum of squares indicates which of the different explanatory variables that contributes the most to the variation in the Structural table.

3.3 Multi-objective optimization

Using MO in LCA was originally suggested by Azapagic in 1999 (Azapagic 1999, Azapagic and Clift 1999a, and Azapagic and Clift 1999b). When dealing with more objectives or goals, there may not be a single solution that is always best, hence there are trade-offs between the different objectives. For instance the most environmentally friendly car is rarely the fastest, too. Hence choosing a best solution depends on preferences for different objectives. This point is illustrated in

Figure 2 where f_1 is speed and f_2 is environmental friendliness. The Pareto front is defined by the solutions that are not dominated by other solutions, i.e. the four white dots in Figure 2.

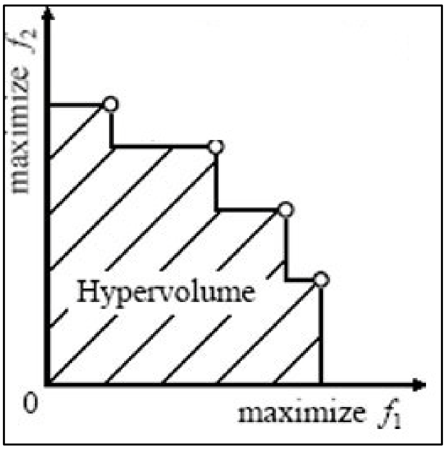

Figure 2. Illustration of trade-off between speed (f_1) and environmental friendliness (f_2) in the MO approach. The Pareto front is the border where no solutions are dominated by other solutions, where as all solutions inside the "Hypervolume" are dominated by solutions on the Pareto front.

Some solutions in Figure 2 are dominated by the solutions placed on the Pareto front in Figure 2, meaning that one or more other solutions are better in all objectives. These dominated solutions are naturally undesired, as there is a better alternative. With three objectives the area in Figure 1 becomes a volume, and with more objectives it becomes a *Hyper*volume which is not practically possible to illustrate.

Compared to the SO method the MO has, at least, one advantage. The SO approach to solve trade-off problems is basically to sum all the objectives with different weights (based on their *assumed* importance) and then choosing the apparently best solution. The SO method however has a serious drawback that makes it an undesirable approach in many optimizations problems. The problem with the SO method is that the LCA practitioner or analyst has to provide very good weights, which are practically impossible to determine. The analyst may have an idea of the overall preference, but to put this into exact weights is difficult, and furthermore the best solution found may not be anything close to the solution that would have been preferred if different solutions had been given to the decision maker.

Traditionally MO has only been practically possible for 2-3 objectives. The new method “Hypervolume Taboo Search” (HETS) which is developed for the present project, makes it possible to investigate far more objectives (up to 25 objectives), by using a faster approximation of the hypervolume compared to traditional methods. This makes HETS highly relevant for LCA which sometimes applies up to 15 different impact categories (Hauschild et al., 2012). The developed HETS algorithms have been tested on a range of different datasets with different number of objectives and problem sizes. It clearly outperforms traditional methods, such as: “Strength Pareto Evolutionary Algorithm” (SPEA-II) (Zitzler et al. 2001); “Non-dominated Sorting Genetic Algorithm” (NSGA-II) (Deb et al. 2002); “Simple Evolutionary Multi-objective Optimizer (SEMO) (Laumanns et al. 2002); or “Set Preference Algorithm for Multi-objective Optimization” (SPAM) (Zitzler, Thiele & Bader 2010) in terms of both speed and performance which can be measured as the quality of the set of solutions achieved. For a further explanation of the quality of the set of solutions achieved see Lundberg-Jensen (2011). With fewer objectives (3-8), the improvement was less significant. Going up to 25 objectives, the improvement was over a factor 50 in computation time. The HETS method and performance is further documented in Lundberg-Jensen (2011).

4 Well-to-wheel study of biodiesel

The functional unit for the LCA is 1000 km driving in a passenger diesel car with a 20 % blend (20B). The use of the passenger diesel car is based on an Ecoinvent process ("*Operation, passenger car, diesel, fleet average 2010/RER U*") which reflects a fleet average in Europe in 2010. The study includes tailpipe emissions, biodiesel production, oil production, alcohol production, and rapeseed production – including specific modeling of fertilizer and pesticide emissions. It is assumed in our study that biogenic CO_2 emissions to atmosphere are balanced out by an equal uptake by growing the crops in the production system (prior to harvest). Hence all biogenic CO_2 emission is accounted with zero impact while CO_2 emission originating from PC diesel is accounted as a net contribution to the CO_2 content of the atmosphere. The baseline scenario of rapeseed fatty acid methyl ester (FAME) is documented in Herrmann et al. (2012). The product system is illustrated in Figure 3.

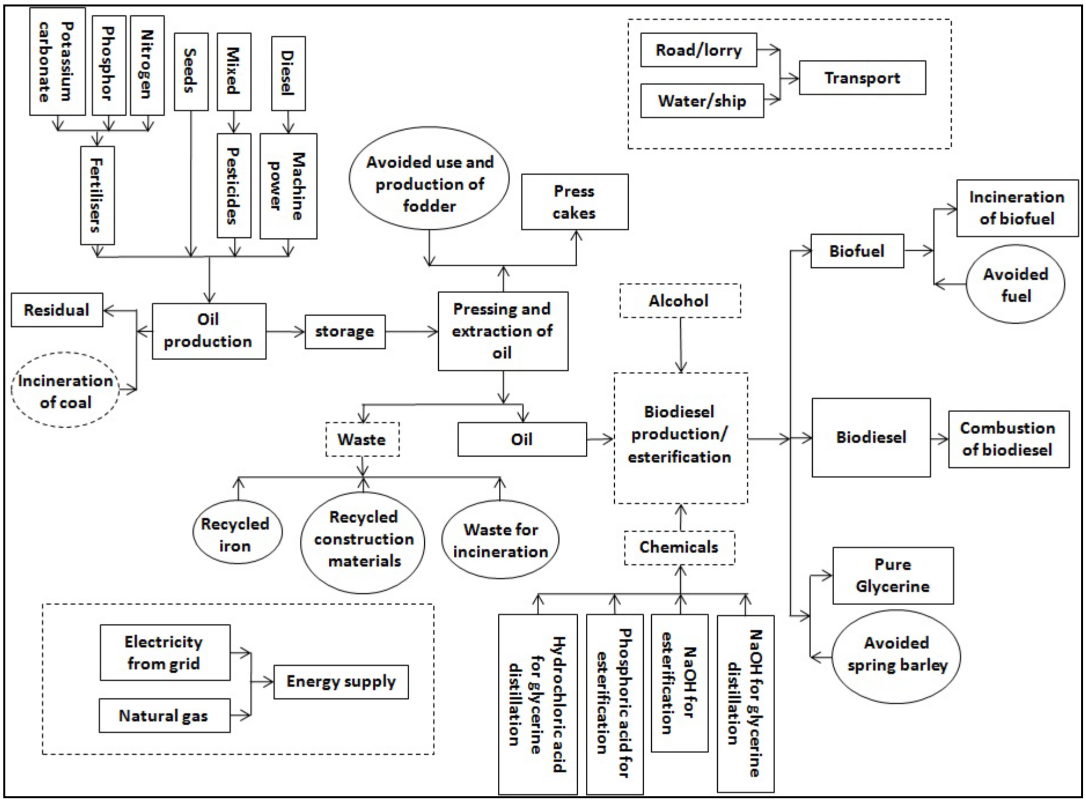

Figure 3 The analysed system for production and combustion of biodiesel for passenger car transport based on different types of diesel (based on Herrmann et al. 2012). Transportation includes road and water transport mainly for transport of feedstock to the pressing and extraction process. The dashed lines illustrate the variables that will or can be changed for creating alternative pathways (PW1-64) – see Table 4.

5 Results and discussion

As described in the method section the selection of the explanatory variables is or can be an on-going process. In the present project we have chosen to demonstrate the Structural approach with the six explanatory variables each with two levels presented in table 3.

Table 3. The six explanatory variables used for illustration of optimization of biodiesel production and use. *Conv.* conventional; *Enz*. Enzymatic; *DK* Denmark; *PL* Poland.

Levels	**Fertilizer mix (fertilizer/manure)**	**Removal of straw for incineration in t/(ha*year)**	**Transesterification process**	**Alcohol**	**Electricity**	**Transport of biodiesel**
Low (-)	0.3/0.7	0	Conv.	BioEt	DK	150 km by lorry
High (+)	0.5/0.5	1	Enz.	PCMe	PL	200 km by lorry and 750 km by ship
Present	0.34/0.66	0.52	Conv.	PCMe	DK	+/-

Main reasons and assumptions for the level settings are outlined in the following. For the use of fertilizer or manure we assume that the crop’s Nitrogen requirement is fixed, hence we only change the ratio between fertilizer and manure. Increasing the use of fertilizer will result in an increased production of this which is highly energy demanding. Approximately there is 3.5 t of straw residual on a land field per year per ha according to Danish Statistics (dst.dk 2011) and some of this can be used for co-incineration in a power plant. We assume that using straw in a power plant will substitute coal in energy ratio approximately 1:1. Either a conventional or an enzymatic transesterification process can be used. Data for the conventional process is from the operation of Emmelev A/S and data for the enzymatic is from Novozymes A/S and Sotoft et al. (2010). The production of bioethanol and petrochemical methanol are based on unit processes from the Ecoinvent database 2.0 (Faist, Heck & Jungbluth 2007). It is assumed that the production of the biodiesel takes place either in Denmark or in Poland which we mainly assume will influence the production of electricity and the transport distance. For further discussion of assumptions and modeling issues we refer to Herrmann et al. (2012).

Furthermore, we considered a range of other explanatory variables, such as use of pesticides, types of oil feedstock, cleaning technology for tailpipe emission, co-product substitution options (e.g. glycerol substituting petrochemical glycerol, wheat for feed, *or* other products (Jørgensen, Bikker &

Herrmann 2012)), and fuel types for heat generation. During the decision process (including Novozymes A/S and Emmelev A/S) on the choice of explanatory variables, levels for these explanatory variables, and the choice of response variables it was decided to use the ones presented in Table 3 and 4 (the response variables in the right side of the table). The rest of the explanatory variables mentioned above were thus considered to be fixed or *ceteris paribus*

5.1 The Structural table

In our case we used SimaPro as the LCA software for modeling our LCA. We used 5 different PWs as fundamental PWs which we successively varied to fit each specific PW setting in the Structural table, Table 4. Second we populated the right side of the Structural table after simulating the specific PW in SimaPro. After using months for collecting data for the five basic PWs it "only" took a week or less to generate the 64 different PWs presented in Table 4 together with the statistical evaluation of these PWs by the use of "R". PW D0 is petrochemical diesel according to the Ecoinvent database 2.0 (Faist, Heck & Jungbluth 2007) and PW1 is biodiesel production based on present conditions according to Herrmann et al. (2012). The full Structural table can be found in Supporting information.

Table 4. The Structural table based on the full factorial 2^6 design (PW 1-64). The full Structural table is to be found in supporting information. *Fert.* Fertilizer; *Alc.* Alcohol; *Elec.* Electricity; *Tran.* transport of biodiesel; *Pre* Present

	Explanatory variables							**Response variables**				
PW	**Fert. mix**	**Use of straw**	**Trans-esteri-fication process**	**Alc.**	**Elec.**	**Tran.**		***Climate change***	***Land Use***	***Respiratory inorganics***	***Human toxicity (carc.)***	***Aquatic eutro-phication N***
D0	NA	NA	NA	NA	NA	NA	=	214.0	0.2	0.0870	1.08E-06	0.06
0	Pre.	Pre.	Pre.	Pre.	Pre.	Pre.	=	57.0	89.8	0.0473	1.50E-06	0.57
1	-	-	Enz.	BioEt	DK	-	=	81.4	101.0	0.0707	1.57E-06	0.55
2	-	-	Enz.	BioEt	DK	+	=	93.2	101.0	0.0798	2.16E-06	0.56
3	-	-	Enz.	BioEt	PL	-	=	82.8	101.0	0.0738	1.64E-06	0.55
4	-	-	Enz.	BioEt	PL	+	=	94.7	101.0	0.0828	2.24E-06	0.56
5	-	-	Enz.	PCMe	DK	-	=	93.0	83.7	0.0483	1.19E-06	0.56
6	-	-	Enz.	PCMe	DK	+	=	105.0	83.7	0.0571	1.85E-06	0.57
7	-	-	Enz.	PCMe	PL	-	=	94.8	83.7	0.0528	1.31E-06	0.56
8	-	-	Enz.	PCMe	PL	+	=	106.0	83.7	0.0617	1.97E-06	0.57
9	-	-	Conv.	BioEt	DK	-	=	78.7	103.0	0.0718	1.86E-06	0.56
…	**…**	**…**	**…**	**…**	**…**	**…**	=	**…**	**…**	**…**	**…**	**…**
64	+	+	Conv.	PCMe	PL	+	=	43.6	83.6	0.0638	2.61E-06	0.59

As the number of explanatory variables of interest or the number of levels for each explanatory variable increases, the number of PWs required being developed increases rapidly; for instance a 10-factor experiment with three levels would require 59049 PWs. This quickly becomes infeasible from a time and resource viewpoint. In this case a *fractional* factorial design can be an alternative to the *full* factorial design. In a fractional factorial design only a subset of the PWs are needed (Montgomery 2005). For example, if we in Figure 1 only had 8 PWs of the 16 possible combinations (illustrated by each corner in the two cubes and the ends of the bracket) then this would be a one half fraction or a 2^{4-1} design which then basically saves half the resources to develop PWs. The trade-off in fractional designs, which becomes more expressed in larger designs, is that some of the lower order interaction effects will be confounded with higher order effects (such as main effects) and if some of these interaction effects are significant then this can potentially blur the interpretation of the resulting statistical model. As the numbers of explanatory variables increases it becomes more complicated to make elegant fractional designs, where as few as possible lower order interaction effects are confounded with higher ordered effects. Some suggestions for these designs can be found in reference books. For example in Montgomery (2005) a 2^{15-11} fractional design can be found which is a 1/2048 fraction of the full design.

5.2 Single-objective optimization

In the following two objectives are analyzed for optimization potentials, namely Climate change potentials (Table 5) and Respiratory inorganics (Table 6). The raw output files from R, which was used to analyse the data, are found in Supporting information. We observed only insignificant interaction effects and hence these were taken out of the final model according to the principle of parsimony (Crawley 2005).

Table 5 and 6 are divided into four columns: the explanatory variables with an indication of the contribution direction, i.e. high (+) or low (-); the effect estimates which are the coefficients in Equation 1 above; the sum of squares which can be interpreted as the variation contribution based on the Structural table; the percent contribution to the variation based on the sum of squares, that is the sum of square for each explanatory variable divided by the total sum of squares. The first row in the table is the intercept or the mean value (μ) in the Equation 1. The intercept is (in this model) a somewhat arbitrary size which is determined by the model we have constructed. In Table 5 we see that changing the ratio of fertilizer versus manure from the low ratio to the high ratio (0.5/0.5) will in response (on average) increase the climate change potential with 13.20 kg CO_2-eq. If we change the removal of straw, from the field and use it for incineration in a power plant which in return will substitute coal, from 0 t/(ha*year) to 1 t/(ha*year), then we will (on average) decrease the climate change potential with 73.6 kg CO_2-eq. If we look at the columns with sum of squares and the percent contribution for sources of variation then we can see that the use of straw is by far the main contributor to the variation of the climate change potential. In a decision support context this indicates where the main potential for optimized production and use of biodiesel is to be found. As indicated in the method section, if the decision maker cannot exercise power over a given explanatory variable then this information might be of less interest. In contrast to "the use of straw from the field" variable we see that the transesterification process or use of electricity in a life cycle perspective, based on our data, contributes with little improvement (or change) to the overall Climate change impact.

Regarding the transesterification process it is important to notice that the conventional process is a mature technology that has been developed over the last decades, while the enzymatic process is a new technology. If the enzymatic processes are developed further, we would expect that there will be a higher potential for improving this technology compared to the already mature and conventional transesterification process. We have made no attempt to predict (or forecast) these potentials. The enzymatic process is based on immobilized enzyme catalysts. Other enzyme processes, including those based on liquid formulated enzyme, could lead to somewhat different results.

Table 5. Optimization potentials of Climate change potential based on effect estimates and sum of squares.

	Effect estimate/ [kg CO_2-eq.]	**Sum of squares**	**Percent (%) contribution**
***Intercept* (μ)**	79.54		
Fert (+)	13.20	2,788	3.0
Straw (+)	-73.55	86,554	92.3
Trans (enz)	2.28	83	0.1
Alc (PCMe)	11.13	1,982	2.1
Electricity (PL)	1.66	44	0.0
Transp (+)	12.06	2,328	2.5

Table 6 presents the optimization potentials for Respiratory inorganics. We see that fertilizer and use of straw contribute to the impact potentials in the same "direction" as for the Climate change potentials, i.e. increasing the use of fertilizer and straw will increase respectively decrease the Respiratory inorganics potentials. On the other hand, we see that where the type of alcohol had relatively little influence on the Climate change potential, then it is the main contributor to the Respiratory inorganics impact potentials. In addition, we see that the type of alcohol contributes in the opposite direction the to the impact potential than for the Climate change potential. This gives some trade-off consideration when deciding on optimized production and use of biodiesel, based on SO. However, one of the main reasons that BioEt relatively to PCMe has such a high effect on the Respiratory inorganics impact category is that in the production of BioEt workers in the sugar cane fields are highly exposed to particles contributing to this impact category. Hence there seems to be a rather large potential to minimize the Respiratory inorganics impact from BioEt (by improved production practices or different shielding technologies) which can reduce the trade-off between the Respiratory inorganics impact category and the Climate change impact category. For further analysis of origin of sources to the different impact categories we refer to Herrmann et al. (2012).

Table 6. Optimization potentials of Respiratory inorganics based on effect estimates and sum of squares.

	Effect estimate/ [kg 2.5PM-eq.]	**Sum of squares**	**Percent (%) contribution**
***Intercept* (μ)**	0.0711844		
Fert (+)	0.0070750	0.0008009	7.0
Straw (+)	-0.0048688	0.0003793	3.3
Trans (enz)	-0.0002000	0.0000006	0.0
Alc (PCMe)	-0.0230313	0.0084870	74.6
Electricity (PL)	0.0043188	0.0002984	2.6
Transp (+)	0.0093750	0.0014062	12.4

When going from the Ad hoc LCA approach to the Structural LCA approach SO becomes possible to use for analyzing data. MO is another optimization method that becomes possible to use when applying the Structural LCA approach. In addition MO can solve some of the above problems that we see with SO of finding the best possible combination, i.e. minimizing the trade-offs when selecting one or more PWs for further investigation.

5.3 Multi-objective optimization

The Pareto optimal front is given in Table 7 by the five PWs which are not dominated by other solutions as indicated in the column “Dominated” by a “No” (while all dominated solutions are indicated by a “Yes”). This number (five) indicates that there is no intuitive solution that dominates all other solutions. At the same time the number of optimal solutions is still a fairly small part of the total solution space. This means that the MO approach is useful not only to find which solutions best represent the Pareto front, but also to actually find the Pareto optimal solutions (unlike when close to all solutions turn out to be optimal in some way). The full Table 7 can be found in Supporting information.

Table 7. The MO approach gives the Pareto optimal front (PW: D0, 17, 21, 25, and 29). *Resp.* Respiratory inorganics; *Htox* Human toxicity (carc.); *Aq. N* Aquatic eutrophication N.

	Explanatory variables							**Response variables**					
PW	**Fert. mix**	**Use of straw**	**Trans-esteri-fication process**	**Alc.**	**Elec.**	**Tran.**		***Climate change***	***Land Use***	***Resp.***	***HTox.***	***Aq. N***	***Domi-nated***
D0	NA	NA	NA	NA	NA	NA	=	214.0	0.2	0.0870	1.08E-06	0.06	No
…	**…**	**…**	**…**	**…**	**…**	**…**	=	**…**	**…**	**…**	**…**	**…**	**…**
17	-	+	Enz.	BioEt	DK	-		10.0	98.7	0.0660	1.41E-06	0.55	No
21	-	+	Enz.	PCMe	PL	-		18.5	81.7	0.0434	1.03E-06	0.56	No
25	-	+	Conv.	BioEt	DK	-		6.3	101.0	0.0670	1.70E-06	0.55	No
29	-	+	Conv.	PCMe	PL	-		15.9	83.4	0.0434	1.30E-06	0.57	No
…	**…**	**…**	**…**	**…**	**…**	**…**	=	**…**	**…**	**…**	**…**	**…**	**…**
61	+	+	Conv.	PCMe	DK	-		29.5	83.6	0.0504	1.88E-06	0.58	Yes
62	+	+	Conv.	PCMe	DK	+		42.1	83.6	0.0600	2.55E-06	0.59	Yes
63	+	+	Conv.	PCMe	PL	-		31.0	83.6	0.0541	1.98E-06	0.58	Yes
64	+	+	Conv.	PCMe	PL	+		43.6	83.6	0.0638	2.61E-06	0.59	Yes

It does not seem likely that with the Ad hoc LCA approach these specific five PW’s (D0, 17, 21, 25, and 29) would have been identified as being optimal solutions. From a decision making point of view we can probably also exclude PW25 since no conventional transesterification that can handle ethanol is likely to be developed in the nearest feature. This can further reduce the Pareto front with one PW. Also considering the supply safety (which is an often mentioned problem for petrochemical fuels) then D0 (petrochemical diesel) can be taken out, too.

5.4 The Ad hoc LCA approach versus the Structural LCA approach

It is important to notice that the Structural LCA approach is not a substitute for the Ad hoc LCA approach but an additional analysis that can be performed given that the data has already been collected (for the Ad hoc LCA approach). In most LCA studies, however, there is normally the option of improving the data quality (for the Ad hoc approach). Given that the LCA practitioner has a fixed amount of resources[2] then it becomes a matter of prioritizing between additional development of the Ad hoc LCA *or*, at the end of a project period, applying the Structural LCA approach with the benefits that can follow from that. This choice will depend on the goal and scope of the LCA. For example, if the LCA is to be used for internal decision support in a company which only has power to change a single explanatory variable then it would be more or less pointless to apply this new Structural LCA approach, since the benefits from the Structural LCA approach mainly relates to a situation where the DM can influence more explanatory variables. In the case where the decision maker can exercise power over more explanatory variables it might become beneficial to apply the Structural LCA approach to identify the explanatory variables that have the highest potentials for reducing the environmental impact in an LCA perspective and to quantify the potentials. In other words, the Structural LCA approach can be used to illuminate where the "low hanging fruits" might be. This can especially be of interest if the LCA is communicated to a broader range of stakeholders, including decision makers at the societal level.

If the LCA is viewed as an on-going process then the potentials for the different explanatory variables change over time as stakeholders/society realize the improvement potentials. For example, if the use of straw is changed from the present situation to a situation where it reaches its limit given by biophysical carbon sequestration constraints and market related constraints, such as competing use of the straw and (missing) economic incentives for use of the straw for power generation, then the magnitude of the potentials for the other explanatory variables will increase.

Potentially some LCA experts and practitioners, based on the Ad hoc LCA approach, could have deduced some of the information presented in Table 5, 6 and 7 by the expert knowledge that they already have. However, it does not seem possible that they in the same manner could have quantified the magnitude of the potentials for each explanatory/response variable and found the Pareto front, as done with the Structural LCA approach.

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[2] E.g. 2 months to perform an LCA study

6 Conclusion

The use of the Structural LCA approach for optimization purposes was demonstrated based on different optimization approaches, such as SO and MO. In addition the structural LCA approach can lead to more transparent LCAs since the explanatory variables[3] which are used to model the LCAs are explicitly presented through the Structural LCA approach. At the same time al other explanatory variables, both known and unknown, are kept constant or *ceteris paribus* which in return gives the reader a clear insight in which are included as changing explanatory variables and which explanatory variables (all others) are kept constant.

Given that there is a fixed amount of resources available for the LCA practitioner it becomes a prioritizing problem whether to apply the Structural LCA approach or not. If the decision maker can only change a single explanatory variable it might not be beneficial to apply the Structural LCA approach. However, if the decision maker (such as decision makers at the societal level) has the power to change more explanatory variables then the Structural LCA approach seems beneficial for quantifying and comparing the potentials for environmental improvement between the different explanatory variables in an LCA system.

In the present analysis of biodiesel in a WTW perspective, and based on SO, we found that the most important explanatory variable for Climate change potential, compared to the other explanatory variables, is the "use of residual straws from fields" which can be used for co-incineration in power plants and hereby substituting coal. For the Respiratory inorganics impact category the use of alcohol contributes the most to the variation and hence improvement potential for this impact category, compared to the other explanatory variables used for optimization potential identification. Based on MO we found the Pareto front consisting of five PWs (D0, 17, 21, 25, and 29) which are not dominated solutions out of the 66 different PWs.

[3] at least the potential most important explanatory variables.

7 Outlook

The suggested Structural LCA approach seems to be a promising approach for searching or screening product systems for environmental optimization potentials. In the presented case the design has been a rather simple full factorial design. The application to more complicated problems or designs, such as fractional designs, nested designs (i.e. where not all levels in an explanatory variable can substitute one another), split plot designs, and/or unbalanced data is an abvious possibility that should be investigated further in the context of LCA.

8 Acknowledgement

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SUPPORTING INFORMATION

Title: **Enabling optimization in LCA from Ad hoc to Structural LCA approach**

- based on a biodiesel well-to-wheel case study

Journal: The International Journal of Life Cycle Assessment

Authors:

Ivan T. Herrmann[a,*], Martin Lundberg-Jensen[b], Henrik Spliid[c], Andreas Jørgensen[a], Thomas Stidsen[b], and Michael Hauschild[a]

*Corresponding author: ivan.t.h.business@gmail.com; P: +45 22756975; F: +45 45933435

[a]Division of Quantitative Sustainability Assessment, Department of Management Engineering, Technical University of Denmark, Produktionstorvet, Building 424, DK-2800, Kgs. Lyngby, Denmark

[b]Division of Management Science, Department of Management Engineering, Technical University of Denmark, Produktionstorvet, Building 424, DK-2800, Kgs. Lyngby, Denmark

[c]Department of Informatics and Mathematical Modeling, Technical University of Denmark, Building 305, DK-2800, Kgs. Lyngby, Denmark

S1: The Structural table with Multi-objective optimization result

The Structural table and multi-objective optimization are explained in the main paper.

S2: Summary and ANOVA output file from "*R*"

The function "Summary" calls the effect coefficients for each explanatory variable from the model constructed. We have used the "lm" model which fits a linear model with normal errors and constant variance. The models have been constructed by using "+" which in this case only gives main effects. Lower ordered effects can be estimate by the use of "*" however almost all variance is explained by the different main effects hence the interaction effects are small and insignificant. ANOVA = Analysis of Variance. Crawley, M.J. 2005, *Statistics: an introduction using R,* J. Wiley, Chichester, West Sussex, England.

S1: The Structural table with Multi-objective optimization result

S1: The Structural table																				
	Explanatory variables														*Response variables*					
PWs	**Agricultural system**				**Biodiesel production system**							**Use phase**			*GWP*	*Land Use*	*Respiratory inorganics*	*Human toxicity (carc.)*	*Aquatic eutrophication N*	*Dominated*
	Fertilizer mix	**Use of straw**	*Use of pesticides*	*Fuel type used in agriculture system*	*Cake substitute*	**Transesterification process**	**Alcohol**	**Electricity**	*Heat*	*Glycerol substitute*	**Transport of biodiesel**	*Type of engine*	*Type of cleaning technology in car*		*kg CO_2-eq/ 1000km*	*m^2 year/ 1000km*	*kg 2.5PM-eq/ 1000km*	*CTUh/ 1000km*	*Kg N/ 1000km*	
PCD	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	**NA**	=	214.0	0.2	0.0870	1.08E-06	0.06	No
0	**Present**	**Present**	**Present**	**Present**	**Present**	**Present**	**Present**	**Present**	**Present**	**Present**	**Present**	**Present**	**Present**	=	57.0	89.8	0.0473	1.50E-06	0.57	Yes
1	-	-	Fixed	Fixed	Fixed	Enz.	BioEt	DK	Fixed	Fixed	-	Fixed	Fixed	=	81.4	101.0	0.0707	1.57E-06	0.55	Yes
2	-	-	Fixed	Fixed	Fixed	Enz.	BioEt	DK	Fixed	Fixed	+	Fixed	Fixed	=	93.2	101.0	0.0798	2.16E-06	0.56	Yes
3	-	-	Fixed	Fixed	Fixed	Enz.	BioEt	PL	Fixed	Fixed	-	Fixed	Fixed	=	82.8	101.0	0.0738	1.64E-06	0.55	Yes
4	-	-	Fixed	Fixed	Fixed	Enz.	BioEt	PL	Fixed	Fixed	+	Fixed	Fixed	=	94.7	101.0	0.0828	2.24E-06	0.56	Yes
5	-	-	Fixed	Fixed	Fixed	Enz.	PCMe	DK	Fixed	Fixed	-	Fixed	Fixed	=	93.0	83.7	0.0483	1.19E-06	0.56	Yes
6	-	-	Fixed	Fixed	Fixed	Enz.	PCMe	DK	Fixed	Fixed	+	Fixed	Fixed	=	105.0	83.7	0.0571	1.85E-06	0.57	Yes
7	-	-	Fixed	Fixed	Fixed	Enz.	PCMe	PL	Fixed	Fixed	-	Fixed	Fixed	=	94.8	83.7	0.0528	1.31E-06	0.56	Yes
8	-	-	Fixed	Fixed	Fixed	Enz.	PCMe	PL	Fixed	Fixed	+	Fixed	Fixed	=	106.0	83.7	0.0617	1.97E-06	0.57	Yes
9	-	-	Fixed	Fixed	Fixed	Conv.	BioEt	DK	Fixed	Fixed	-	Fixed	Fixed	=	78.7	103.0	0.0718	1.86E-06	0.56	Yes
10	-	-	Fixed	Fixed	Fixed	Conv.	BioEt	DK	Fixed	Fixed	+	Fixed	Fixed	=	90.8	103.0	0.0810	2.46E-06	0.57	Yes
11	-	-	Fixed	Fixed	Fixed	Conv.	BioEt	PL	Fixed	Fixed	-	Fixed	Fixed	=	80.2	103.0	0.0754	1.95E-06	0.56	Yes
12	-	-	Fixed	Fixed	Fixed	Conv.	BioEt	PL	Fixed	Fixed	+	Fixed	Fixed	=	92.2	103.0	0.0846	2.55E-06	0.57	Yes
13	-	-	Fixed	Fixed	Fixed	Conv.	PCMe	DK	Fixed	Fixed	-	Fixed	Fixed	=	92.0	85.5	0.0484	1.46E-06	0.57	Yes
14	-	-	Fixed	Fixed	Fixed	Conv.	PCMe	DK	Fixed	Fixed	+	Fixed	Fixed	=	105.0	85.5	0.0581	2.09E-06	0.59	Yes
15	-	-	Fixed	Fixed	Fixed	Conv.	PCMe	PL	Fixed	Fixed	-	Fixed	Fixed	=	93.5	85.5	0.0522	1.56E-06	0.57	Yes
16	-	-	Fixed	Fixed	Fixed	Conv.	PCMe	PL	Fixed	Fixed	+	Fixed	Fixed	=	106.0	85.5	0.0618	2.19E-06	0.59	Yes
17	-	+	Fixed	Fixed	Fixed	Enz.	BioEt	DK	Fixed	Fixed	-	Fixed	Fixed	=	10.0	98.7	0.0660	1.41E-06	0.55	No
18	-	+	Fixed	Fixed	Fixed	Enz.	BioEt	DK	Fixed	Fixed	+	Fixed	Fixed	=	21.8	98.7	0.0751	2.01E-06	0.56	Yes
19	-	+	Fixed	Fixed	Fixed	Enz.	BioEt	PL	Fixed	Fixed	-	Fixed	Fixed	=	12.2	98.7	0.0714	1.55E-06	0.55	Yes
20	-	+	Fixed	Fixed	Fixed	Enz.	BioEt	PL	Fixed	Fixed	+	Fixed	Fixed	=	24.1	98.7	0.0805	2.15E-06	0.56	Yes
21	-	+	Fixed	Fixed	Fixed	Enz.	PCMe	DK	Fixed	Fixed	-	Fixed	Fixed	=	18.5	81.7	0.0434	1.03E-06	0.56	No
22	-	+	Fixed	Fixed	Fixed	Enz.	PCMe	DK	Fixed	Fixed	+	Fixed	Fixed	=	30.2	81.7	0.0522	1.69E-06	0.57	Yes
23	-	+	Fixed	Fixed	Fixed	Enz.	PCMe	PL	Fixed	Fixed	-	Fixed	Fixed	=	20.4	81.7	0.0476	1.15E-06	0.56	Yes
24	-	+	Fixed	Fixed	Fixed	Enz.	PCMe	PL	Fixed	Fixed	+	Fixed	Fixed	=	32.0	81.7	0.0567	1.81E-06	0.57	Yes
25	-	+	Fixed	Fixed	Fixed	Conv.	BioEt	DK	Fixed	Fixed	-	Fixed	Fixed	=	6.3	101.0	0.0670	1.70E-06	0.55	No
26	-	+	Fixed	Fixed	Fixed	Conv.	BioEt	DK	Fixed	Fixed	+	Fixed	Fixed	=	18.3	101.0	0.0762	2.31E-06	0.57	Yes
27	-	+	Fixed	Fixed	Fixed	Conv.	BioEt	PL	Fixed	Fixed	-	Fixed	Fixed	=	7.8	101.0	0.0706	1.80E-06	0.55	Yes
28	-	+	Fixed	Fixed	Fixed	Conv.	BioEt	PL	Fixed	Fixed	+	Fixed	Fixed	=	19.8	101.0	0.0799	2.40E-06	0.57	Yes
29	-	+	Fixed	Fixed	Fixed	Conv.	PCMe	DK	Fixed	Fixed	-	Fixed	Fixed	=	15.9	83.4	0.0434	1.30E-06	0.57	No
30	-	+	Fixed	Fixed	Fixed	Conv.	PCMe	DK	Fixed	Fixed	+	Fixed	Fixed	=	28.6	83.4	0.0531	1.93E-06	0.58	Yes
31	-	+	Fixed	Fixed	Fixed	Conv.	PCMe	PL	Fixed	Fixed	-	Fixed	Fixed	=	17.4	83.4	0.0472	1.39E-06	0.57	Yes
32	-	+	Fixed	Fixed	Fixed	Conv.	PCMe	PL	Fixed	Fixed	+	Fixed	Fixed	=	30.1	83.4	0.0568	2.03E-06	0.58	Yes
33	+	-	Fixed	Fixed	Fixed	Enz.	BioEt	DK	Fixed	Fixed	-	Fixed	Fixed	=	94.2	101.0	0.0773	2.12E-06	0.55	Yes
34	+	-	Fixed	Fixed	Fixed	Enz.	BioEt	DK	Fixed	Fixed	+	Fixed	Fixed	=	106.0	101.0	0.0864	2.71E-06	0.57	Yes
35	+	-	Fixed	Fixed	Fixed	Enz.	BioEt	PL	Fixed	Fixed	-	Fixed	Fixed	=	96.4	101.0	0.0826	2.25E-06	0.55	Yes
36	+	-	Fixed	Fixed	Fixed	Enz.	BioEt	PL	Fixed	Fixed	+	Fixed	Fixed	=	108.0	101.0	0.0971	2.85E-06	0.57	Yes
37	+	-	Fixed	Fixed	Fixed	Enz.	PCMe	DK	Fixed	Fixed	-	Fixed	Fixed	=	106.0	83.9	0.0551	1.76E-06	0.57	Yes
38	+	-	Fixed	Fixed	Fixed	Enz.	PCMe	DK	Fixed	Fixed	+	Fixed	Fixed	=	118.0	83.9	0.0639	2.42E-06	0.58	Yes
39	+	-	Fixed	Fixed	Fixed	Enz.	PCMe	PL	Fixed	Fixed	-	Fixed	Fixed	=	108.0	83.9	0.0596	1.88E-06	0.57	Yes
40	+	-	Fixed	Fixed	Fixed	Enz.	PCMe	PL	Fixed	Fixed	+	Fixed	Fixed	=	120.0	83.9	0.0685	2.54E-06	0.58	Yes
41	+	-	Fixed	Fixed	Fixed	Conv.	BioEt	DK	Fixed	Fixed	-	Fixed	Fixed	=	91.7	103.0	0.0784	2.42E-06	0.56	Yes
42	+	-	Fixed	Fixed	Fixed	Conv.	BioEt	DK	Fixed	Fixed	+	Fixed	Fixed	=	104.0	103.0	0.0876	3.02E-06	0.57	Yes
43	+	-	Fixed	Fixed	Fixed	Conv.	BioEt	PL	Fixed	Fixed	-	Fixed	Fixed	=	93.1	103.0	0.0820	2.51E-06	0.56	Yes
44	+	-	Fixed	Fixed	Fixed	Conv.	BioEt	PL	Fixed	Fixed	+	Fixed	Fixed	=	105.0	103.0	0.0913	3.11E-06	0.57	Yes
45	+	-	Fixed	Fixed	Fixed	Conv.	PCMe	DK	Fixed	Fixed	-	Fixed	Fixed	=	106.0	85.7	0.0554	2.05E-06	0.58	Yes
46	+	-	Fixed	Fixed	Fixed	Conv.	PCMe	DK	Fixed	Fixed	+	Fixed	Fixed	=	118.0	85.7	0.0651	2.68E-06	0.59	Yes
47	+	-	Fixed	Fixed	Fixed	Conv.	PCMe	PL	Fixed	Fixed	-	Fixed	Fixed	=	107.0	85.7	0.0591	2.14E-06	0.58	Yes
48	+	-	Fixed	Fixed	Fixed	Conv.	PCMe	PL	Fixed	Fixed	+	Fixed	Fixed	=	120.0	85.7	0.0688	2.77E-06	0.59	Yes
49	+	+	Fixed	Fixed	Fixed	Enz.	BioEt	DK	Fixed	Fixed	-	Fixed	Fixed	=	22.7	98.9	0.0729	1.97E-06	0.55	Yes
50	+	+	Fixed	Fixed	Fixed	Enz.	BioEt	DK	Fixed	Fixed	+	Fixed	Fixed	=	34.6	98.9	0.0817	2.56E-06	0.56	Yes
51	+	+	Fixed	Fixed	Fixed	Enz.	BioEt	PL	Fixed	Fixed	-	Fixed	Fixed	=	25.0	98.9	0.0779	2.10E-06	0.55	Yes
52	+	+	Fixed	Fixed	Fixed	Enz.	BioEt	PL	Fixed	Fixed	+	Fixed	Fixed	=	36.9	98.9	0.0870	2.70E-06	0.56	Yes
53	+	+	Fixed	Fixed	Fixed	Enz.	PCMe	DK	Fixed	Fixed	-	Fixed	Fixed	=	31.8	81.9	0.0502	1.60E-06	0.56	Yes
54	+	+	Fixed	Fixed	Fixed	Enz.	PCMe	DK	Fixed	Fixed	+	Fixed	Fixed	=	43.5	81.9	0.0590	2.26E-06	0.58	Yes
55	+	+	Fixed	Fixed	Fixed	Enz.	PCMe	PL	Fixed	Fixed	-	Fixed	Fixed	=	33.7	81.9	0.0547	1.72E-06	0.57	Yes
56	+	+	Fixed	Fixed	Fixed	Enz.	PCMe	PL	Fixed	Fixed	+	Fixed	Fixed	=	45.4	81.9	0.0636	2.38E-06	0.58	Yes
57	+	+	Fixed	Fixed	Fixed	Conv.	BioEt	DK	Fixed	Fixed	-	Fixed	Fixed	=	19.2	101.0	0.0736	2.26E-06	0.56	Yes
58	+	+	Fixed	Fixed	Fixed	Conv.	BioEt	DK	Fixed	Fixed	+	Fixed	Fixed	=	31.3	101.0	0.0829	2.86E-06	0.57	Yes
59	+	+	Fixed	Fixed	Fixed	Conv.	BioEt	PL	Fixed	Fixed	-	Fixed	Fixed	=	20.7	101.0	0.0773	2.35E-06	0.56	Yes
60	+	+	Fixed	Fixed	Fixed	Conv.	BioEt	PL	Fixed	Fixed	+	Fixed	Fixed	=	32.7	101.0	0.0865	2.96E-06	0.57	Yes
61	+	+	Fixed	Fixed	Fixed	Conv.	PCMe	DK	Fixed	Fixed	-	Fixed	Fixed	=	29.5	83.6	0.0504	1.88E-06	0.58	Yes
62	+	+	Fixed	Fixed	Fixed	Conv.	PCMe	DK	Fixed	Fixed	+	Fixed	Fixed	=	42.1	83.6	0.0600	2.52E-06	0.59	Yes
63	+	+	Fixed	Fixed	Fixed	Conv.	PCMe	PL	Fixed	Fixed	-	Fixed	Fixed	=	31.0	83.6	0.0541	1.98E-06	0.58	Yes
64	+	+	Fixed	Fixed	Fixed	Conv.	PCMe	PL	Fixed	Fixed	+	Fixed	Fixed	=	43.6	83.6	0.0638	2.61E-06	0.59	Yes

```
R version 2.13.0 (2011-04-13)
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[Previously saved workspace restored]

> x <- read.table('C:\\Users\\ithe\\Desktop\\Opti.txt', header=T)
> attach(x)
> names(x)
 [1] "Fert"        "Straw"       "Pest"        "Fueltype"    "Cake"        "Trans"       "Alc"
        "Electricity" "Heat"        "Glyce"
[11] "Transp"      "Engi"        "Tech"        "X."          "GWP"         "Land"        "Resp
"        "ToxH"        "EutroN"
> modelGWP = lm(GWP ~ Fert + Straw + Trans + Alc + Electricity + Transp)
> modelLand = lm(Land ~ Fert + Straw + Trans + Alc + Electricity + Transp)
> modelResp = lm(Resp ~ Fert + Straw + Trans + Alc + Electricity + Transp)
> modelToxH = lm(ToxH ~ Fert + Straw + Trans + Alc + Electricity + Transp)
> modelEutroN = lm(EutroN ~ Fert + Straw + Trans + Alc + Electricity + Transp)
> summary(modelGWP)

Call:
lm(formula = GWP ~ Fert + Straw + Trans + Alc + Electricity +
    Transp)

Residuals:
    Min      1Q  Median      3Q     Max
-1.4688 -0.8297 -0.2844  0.4969  2.4000

Coefficients:
              Estimate Std. Error  t value Pr(>|t|)
(Intercept)    79.5438     0.3895  204.206  < 2e-16 ***
Fert+          13.2000     0.2945   44.829  < 2e-16 ***
Straw+        -73.5500     0.2945 -249.784  < 2e-16 ***
TransEnz.       2.2750     0.2945    7.726 1.96e-10 ***
AlcPCMe        11.1312     0.2945   37.803  < 2e-16 ***
ElectricityPL   1.6625     0.2945    5.646 5.42e-07 ***
Transp+        12.0625     0.2945   40.966  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.178 on 57 degrees of freedom
Multiple R-squared: 0.9992,     Adjusted R-squared: 0.9991
F-statistic: 1.127e+04 on 6 and 57 DF,  p-value: < 2.2e-16

> anova(modelGWP)
Analysis of Variance Table

Response: GWP
            Df Sum Sq Mean Sq   F value    Pr(>F)
Fert         1   2788    2788  2009.603 < 2.2e-16 ***
Straw        1  86554   86554 62391.849 < 2.2e-16 ***
Trans        1     83      83    59.693 1.961e-10 ***
Alc          1   1982    1982  1429.060 < 2.2e-16 ***
Electricity  1     44      44    31.878 5.424e-07 ***
Transp       1   2328    2328  1678.175 < 2.2e-16 ***
Residuals   57     79       1
---
```

```
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
> summary(modelLand)

Call:
lm(formula = Land ~ Fert + Straw + Trans + Alc + Electricity +
    Transp)

Residuals:
     Min       1Q   Median       3Q      Max
-0.18750 -0.09375  0.00000  0.08750  0.18750

Coefficients:
                Estimate Std. Error  t value Pr(>|t|)
(Intercept)    1.029e+02  3.794e-02 2712.129  < 2e-16 ***
Fert+          1.250e-01  2.868e-02    4.359 5.53e-05 ***
Straw+        -2.075e+00  2.868e-02  -72.358  < 2e-16 ***
TransEnz.     -1.925e+00  2.868e-02  -67.127  < 2e-16 ***
AlcPCMe       -1.728e+01  2.868e-02 -602.400  < 2e-16 ***
ElectricityPL -1.868e-15  2.868e-02    0.000        1
Transp+       -1.696e-15  2.868e-02    0.000        1
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.1147 on 57 degrees of freedom
Multiple R-squared: 0.9998,     Adjusted R-squared: 0.9998
F-statistic: 6.211e+04 on 6 and 57 DF,  p-value: < 2.2e-16

> anova(modelLand)
Analysis of Variance Table

Response: Land
            Df Sum Sq Mean Sq  F value    Pr(>F)
Fert         1    0.2     0.2     19.0 5.527e-05 ***
Straw        1   68.9    68.9   5235.6 < 2.2e-16 ***
Trans        1   59.3    59.3   4506.0 < 2.2e-16 ***
Alc          1 4774.8  4774.8 362885.6 < 2.2e-16 ***
Electricity  1    0.0     0.0      0.0         1
Transp       1    0.0     0.0      0.0         1
Residuals   57    0.8     0.0
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
> summary(modelResp)

Call:
lm(formula = Resp ~ Fert + Straw + Trans + Alc + Electricity +
    Transp)

Residuals:
       Min         1Q     Median         3Q        Max
-0.0018781 -0.0003156 -0.0000406  0.0002484  0.0053469

Coefficients:
                Estimate Std. Error t value Pr(>|t|)
(Intercept)    0.0711844  0.0002940  242.08   <2e-16 ***
Fert+          0.0070750  0.0002223   31.83   <2e-16 ***
Straw+        -0.0048688  0.0002223  -21.90   <2e-16 ***
TransEnz.     -0.0002000  0.0002223   -0.90    0.372
AlcPCMe       -0.0230313  0.0002223 -103.61   <2e-16 ***
ElectricityPL  0.0043188  0.0002223   19.43   <2e-16 ***
Transp+        0.0093750  0.0002223   42.18   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.0008891 on 57 degrees of freedom
Multiple R-squared: 0.9961,     Adjusted R-squared: 0.9956
F-statistic:  2398 on 6 and 57 DF,  p-value: < 2.2e-16

> anova(modelResp)
Analysis of Variance Table

Response: Resp
            Df    Sum Sq   Mean Sq    F value Pr(>F)
Fert         1 0.0008009 0.0008009  1013.0958 <2e-16 ***
```

```
Straw        1 0.0003793 0.0003793   479.7694 <2e-16 ***
Trans        1 0.0000006 0.0000006     0.8096  0.372
Alc          1 0.0084870 0.0084870 10735.7563 <2e-16 ***
Electricity  1 0.0002984 0.0002984   377.4972 <2e-16 ***
Transp       1 0.0014062 0.0014062  1778.8535 <2e-16 ***
Residuals   57 0.0000451 0.0000008
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
> summary(modelToxH)

Call:
lm(formula = ToxH ~ Fert + Straw + Trans + Alc + Electricity +
    Transp)

Residuals:
       Min         1Q     Median         3Q        Max
-4.922e-08 -1.289e-08 -3.438e-09  1.641e-08  3.703e-08

Coefficients:
                Estimate Std. Error t value Pr(>|t|)
(Intercept)    1.826e-06  6.869e-09  265.89   <2e-16 ***
Fert+          5.697e-07  5.192e-09  109.71   <2e-16 ***
Straw+        -1.534e-07  5.192e-09  -29.55   <2e-16 ***
TransEnz.     -2.672e-07  5.192e-09  -51.46   <2e-16 ***
AlcPCMe       -3.553e-07  5.192e-09  -68.43   <2e-16 ***
ElectricityPL  1.072e-07  5.192e-09   20.64   <2e-16 ***
Transp+        6.228e-07  5.192e-09  119.94   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 2.077e-08 on 57 degrees of freedom
Multiple R-squared: 0.9984,     Adjusted R-squared: 0.9982
F-statistic:  5842 on 6 and 57 DF,  p-value: < 2.2e-16

> anova(modelToxH)
Analysis of Variance Table

Response: ToxH
            Df     Sum Sq    Mean Sq  F value    Pr(>F)
Fert         1 5.1927e-12 5.1927e-12 12037.22 < 2.2e-16 ***
Straw        1 3.7670e-13 3.7670e-13   873.20 < 2.2e-16 ***
Trans        1 1.1422e-12 1.1422e-12  2647.80 < 2.2e-16 ***
Alc          1 2.0200e-12 2.0200e-12  4682.46 < 2.2e-16 ***
Electricity  1 1.8380e-13 1.8380e-13   426.13 < 2.2e-16 ***
Transp       1 6.2063e-12 6.2063e-12 14386.91 < 2.2e-16 ***
Residuals   57 2.4600e-14 4.0000e-16
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
> summary(modelEutroN)

Call:
lm(formula = EutroN ~ Fert + Straw + Trans + Alc + Electricity +
    Transp)

Residuals:
       Min         1Q     Median         3Q        Max
-0.0057812 -0.0026562 -0.0001562  0.0023438  0.0054688

Coefficients:
                Estimate Std. Error t value Pr(>|t|)
(Intercept)    0.5570313  0.0010632 523.935  < 2e-16 ***
Fert+          0.0053125  0.0008037   6.610 1.42e-08 ***
Straw+        -0.0021875  0.0008037  -2.722   0.0086 **
TransEnz.     -0.0096875  0.0008037 -12.054  < 2e-16 ***
AlcPCMe        0.0153125  0.0008037  19.053  < 2e-16 ***
ElectricityPL  0.0003125  0.0008037   0.389   0.6988
Transp+        0.0121875  0.0008037  15.165  < 2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.003215 on 57 degrees of freedom
Multiple R-squared: 0.9327,     Adjusted R-squared: 0.9256
F-statistic: 131.6 on 6 and 57 DF,  p-value: < 2.2e-16
```

```
> anova(modelEutroN)
Analysis of Variance Table

Response: EutroN
            Df    Sum Sq   Mean Sq  F value    Pr(>F)    
Fert         1 0.0004516 0.0004516  43.6950 1.416e-08 ***
Straw        1 0.0000766 0.0000766   7.4085  0.008596 ** 
Trans        1 0.0015016 0.0015016 145.2971 < 2.2e-16 ***
Alc          1 0.0037516 0.0037516 363.0159 < 2.2e-16 ***
Electricity  1 0.0000016 0.0000016   0.1512  0.698846    
Transp       1 0.0023766 0.0023766 229.9655 < 2.2e-16 ***
Residuals   57 0.0005891 0.0000103                      
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
>
```

Appendix E: Assessing the greenhouse gas emissions from poultry fat biodiesel

Authors: Andreas Jørgensen, Paul Bikker, and Ivan T. Herrmann

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Assessing the greenhouse gas emissions from poultry fat biodiesel

Andreas Jørgensen [a,*], Paul Bikker [b], Ivan T. Herrmann [a]

[a] Department of Management Engineering, Section of Quantitative Sustainability Assessment, Technical University of Denmark, DK-2800, Kgs. Lyngby, Denmark
[b] Wageningen UR Livestock Research, 6708 WC Wageningen, The Netherlands

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ABSTRACT

This article attempts to answer the question: What will most likely happen in terms of emitted greenhouse gases if the use of poultry fat for making biodiesel used in transportation is increased? Through a well-to-wheel assessment, several different possible scenarios are assessed, showing that under average conditions, the use of poultry fat biodiesel instead of diesel leads to a slight reduction (6%) in greenhouse gas emissions. The analysis shows that poultry fat is already used for different purposes and using poultry fat for biodiesel will therefore remove the poultry fat from its original use. This implies that even though the use of biodiesel is assumed to displace petrochemical diesel, the 'original user' of the poultry fat will have to find a substitute, whose production leads to a greenhouse gas emissions comparable to what is saved through driving on poultry fat biodiesel rather than petrochemical diesel. Given that it is the production of the substitute for the poultry fat which mainly eliminates the benefit from using poultry fat for biodiesel, it is argued that whenever assessing the greenhouse gas emissions from biodiesel made from by-products (such as rendered animal fats, used cooking oil, etc.) it is very important to include the oil's alternative use in the assessment.

1. Introduction

Biodiesel has often been mentioned as a fuel with the potential for combating climate change. Many studies have been made to assess whether the substitution of petrochemical diesel with biodiesel will in fact lead to lower greenhouse gas (GHG) emissions over their complete life cycle, and the results depend, among others, on the oil used for the biodiesel production. One group of oils used for biodiesel is 'by-product' oils (BPO), which as the name indicate are oils produced as a by-product in various processes. BPO comprise for example used vegetable oils, used cooking oils, animal fat from rendering of animal carcasses, and yellow grease. Several studies have addressed environmental issues related to biodiesel from BPO (Beer et al., 2007; Jensen et al., 2007; López et al., 2010; Morais et al., 2010; Montrimaite et al., 2010; Nelson and Schrock, 2006; Niederl and Narodoslawsky, 2004; Ozata et al., 2008; Peiro et al., 2010; Pleanjai et al., 2009; UK Department for Transport, 2008; US EPA, 2010; Xunmin et al., 2009; Zah et al., 2007), however, none of these have addressed the GHG emissions from the use of poultry fat (PF) for biodiesel. The purpose of this study is to assess what will most likely happen in terms of emitted GHG if it is chosen to use PF for making biodiesel used in transportation. In order to answer this question, a case study focusing on well-to-wheel GHG emissions caused by the production and use of 1 kg of PF biodiesel in the US, is performed.

2. Method

This study follows the steps in a life cycle assessment (LCA), being goal and scope definition, inventory, and impact assessment (JRC, 2010). These steps will be addressed below.

2.1. Goal and scope definition

The purpose of this study is as noted to answer the question: What will happen in terms of emitted GHG if PF is used for making biodiesel used in transportation? When 'something happens' it can be understood as a change from a baseline situation. Thus, by this question we are interested in assessing the difference in GHG emissions from the baseline scenario in comparison to a 'new situation', which can be expressed as the difference in terms of emitted GHGs between a situation where PF is used for production and use of biodiesel and the baseline situation where it is not.

An obvious obstacle in answering this question is, however, that at least one of the mentioned situations are going to be counterfactual, and that the assessment therefore by nature will have a speculative character. Yet, if we are interested in answering the

* Corresponding author. Tel.: +45 4525 4443.
E-mail addresses: aj@man.dtu.dk (A. Jørgensen), paul.bikker@wur.nl (P. Bikker), ithe@man.dtu.dk (I.T. Herrmann).

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question stated above, this is an issue which cannot be avoided by any methodological 'tricks'.

As the GHG emissions arise from the processes included in the assessment, to identify the change in GHG emissions the processes that change as a result of the use of PF for biodiesel need to be identified. The processes that change will depend on production and market conditions. In this assessment, it was chosen to use existing production and market conditions in the US. Given that these change relatively rapidly over time in the biodiesel sector, the assessment should only be considered valid within the next few years.

In the following the changes that are expected most likely to occur as a result of the use of PF for biodiesel, are outlined.

Literature on what PF is used for, if not for biodiesel is scarce. Literature suggests that animal fats in general are most likely used in the feed industry (López et al., 2010; Meeker, 2009), and that PF is often used in poultry feed (Firman, 2006; Groschen, 2002). Thus, in this assessment it is assumed that if PF is not used for biodiesel, it will be used in poultry feed. In this connection a question which arises is whether an increase in demand for PF from biodiesel producers will simply increase the production of PF to meet the new demand or whether its use for biodiesel will incline feed producers to find a substitute. We assume that due to the low value of PF in comparison to the meat production, an increase in the demand and thereby price of PF will not lead the poultry farmers to increase their production of poultry and thereby PF. For other rendered fats, this assumption is supported elsewhere (Stiefelmeyer et al., 2006).

It is thus assumed that if the PF is used for biodiesel, this will most likely lead feed producers to find a substitute rather than make poultry farmers produce more poultry. This implies that as no changes in the production of poultry are expected no emissions related to the production of poultry are included in the assessment.

Biodiesel is, however, not made from oil alone, but depends also on inputs of methanol and various chemicals and energy. Biodiesel may be made through different processes, which will affect both needed inputs and produced outputs. Two options are considered; a batch transesterification process of PF and methanol using potassium hydroxide as a catalyst; and a similar process but including an esterification step before the transesterification where the free fatty acid content in the PF is converted to biodiesel using sulfuric acid as a catalyst. Regardless of the approach used, we have assumed that the use of methanol, chemicals and energy will result in additional production of these goods by marginal[1] producers. In most cases these are considered to be the average producers, as differences in GHG emissions between marginal and average technologies are assumed to be small, however, when it comes to electricity, this assumption does not hold (Ekvall and Weidema, 2004). Due to the complexity in identifying the marginal electricity production (Lund et al., 2010) two different scenarios are considered; one where the electricity is based on coal, the other on natural gas.

Both biodiesel processes result in the production of biodiesel, glycerol and some 'lost biofuel', which is mainly a mix of biodiesel, glycerol and ethanol (Burton, 2011).

With regards to the outputs from the biodiesel production, the production of biodiesel is assumed to be used for transportation instead of petrochemical diesel, displacing both its production and use.

The glycerol is more difficult, as it is somewhat unclear what additional glycerol on the market would imply. First of all, it may substitute petrochemical glycerol (Malca and Friere, 2011; JRC, 2007). This scenario is, however, not considered very likely, due to the large production of glycerol from biodiesel production and the relatively low demand for petrochemical glycerol (JRC, 2007). Within the chemical industry the most economically attractive use has been claimed to be the production of propylene glycol (PG) (1,2 and 1,3-propanediol) from glycerol (Pagliaro and Rossi, 2010; JRC, 2007). A problem with this assumption is, however, that to our knowledge very few companies perform this process today, and given the short time span of the assessment, it is questionable whether the production capacity will increase within this period. Purified glycerol may also be used in the feed industry (Malca and Friere, 2011; Bauen et al., 2010) substituting energy from carbohydrates. Finally, it may also be used unpurified in boilers, substituting petrochemical fuel (JRC, 2007), but this solution is not very economically attractive (JRC, 2007). Which of these can be considered the most likely scenario, is difficult to assess. We have chosen to consider the use of glycerol in the production of PG or as feed in the main scenarios. However, to assess the importance of these assumptions about glycerol in more depth, the two other possibilities are included in the discussion of the results.

The mentioned 'lost biofuel' is assumed to be used in an industrial boiler (Burton, 2011), thereby displacing the production and use of fuel oil.

To summarize, the most likely changes incurred if PF is used for biodiesel in comparison to the baseline situation where it is not, are found to be the following:

The outlined 2 different ways of producing biodiesel, 2 ways of utilizing glycerol from biodiesel, and the 2 different electricity supplies in total make up 8 possible scenarios, all of which are included in the following assessment.

When calculating the GHG emissions related to these changes, we are not using the often used 'accounting principle' of 'biogenic' GHG emissions. Even though this is fully possible to utilize and very practical in many situations, it will in this case easily give some confusion in relation to the set boundaries. Rather, to keep the assessment as simple as possible, we will simply focus on the emissions and absorptions of GHGs that the changes outlined above will create. It should, however, be emphasized that regardless which 'accounting principles' are used, the results should obviously be the same.

2.2. Inventory and impact assessment

Below, each of the listed changes in Table 1, will be described in more detail in order to assess the resulting changes in GHG[2] emissions. Changes in transportation are considered for each change.

2.2.1. Increased production of PF biodiesel (1)

As mentioned above, two different PF biodiesel production processes are considered. One is a common batch transesterification process using potassium hydroxide as a catalyst. Due to the content of free fatty acids (FFA) in the PF, this process results in some soap formation, which in our case company is washed out with the waste water (Burton, 2011). The other process is similar, but includes an esterification process of the PF before the transesterification step. The esterification process is made to esterify the FFA to biodiesel, thereby avoiding the soap formation, using sulfuric acid as a catalyst.

Data for the transesterification process is based on data obtained from Piedmont Biofuels (Burton, 2011), a biodiesel producer

[1] The marginal product is defined as the product which will change in supply due to changes in demand.

[2] The characterization factors for GHGs are based on the IPCC fourth assessment revision report (Fosters and Ramaswamy, 2007).

Table 1
Changes created by the use of PF for biodiesel. Numbers refer to the sections below where the changes are described and the resulting GHG emissions calculated.

Baseline	New situation	Change
- Use of PF in feed	- Use of PF in the production of biodiesel	Increased production of biodiesel (1). Increased production of substitutes in feed (2)
- Driving on diesel	- Driving on biodiesel	Decreased production of diesel (increased production of biodiesel included above) and changes in the emission profile of car (3)
- Use of petrochemical PG, *or* use of energy feed	- Use of PG made from biodiesel glycerol, *or* use of glycerol from the production of biodiesel	Decreased production of petrochemical PG and increase in the production of PG from biodiesel glycerol (4), *or* decreased production of energy feed (5)
- Use of light fuel in industrial boiler	- Use of lost biofuel from the production of biodiesel	Decreased production of light fuel oil for industrial boiler and change in the emission profile of boiler (3).

operating in Pittsboro, NC, in the US. As this facility does not include an esterification process, the data for this is based on literature (Canakci and Van Gerpen, 2003). Also, as the facility does not include a facility for distillation of the glycerol, data from a biodiesel producer in Denmark (Gordon, 2011), was used for the scenarios demanding pure glycerol. Piedmont Biofuels has not had any problems keeping below the sulfur content limits, and no desulphurization process is therefore included. The resulting GHG emissions are calculated on the basis of standard process data (Ecoinvent, 2007) (Table 2).

Transportation of the PF to the biodiesel facility is assumed to be the same as the transport would have been if the PF had been transported to the feed producing facilities. The same is the case for the transport of the PF biodiesel to the customers, which is assumed to be the same as the transport of the petrochemical diesel from the refineries to the end customers in the baseline scenario. In the same way, the transportation of glycerol and lost biofuel to the end consumers are not considered to lead to any additional transportation, too. The added transport above therefore relates only to the transportation of the included chemicals and methanol.

Table 2
Inputs and outputs from the production of PF biodiesel and resulting GHG emissions. The two emissions for electricity refer to power produced from coal and natural gas. 'Est.' implies that the value is estimated, and 'calc.' that the value is calculated on the basis of stoichiometry.

Inputs	Quantity	GHG emission (kg CO_2 eq.)
Transesterification		
PF	1.16 kg	
Methanol	0.224 kg	0.167
Potassium hydroxide	0.00996 kg	0.0197
Electricity	0.157 kWh	0.187; 0.107
Process water	0.782 kg	0.000249
Biodiesel plant	8e-10 pcs (Est.)	0.00197
Transportation of chemicals and methanol	48 kg*km (Est.)	0.00929
Glycerol purification		
Sodium hydroxide (50%)	0.00413 kg	0.00478
Hydrochloric acid (30%)	0.00785 kg	0.00721
Process steam	0.153 MJ	0.0124
Electricity	0.004 kWh	0.00476; 0.0027
Esterification (of 2 % FFA)		
Sulfuric acid	1.23e-3 kg	1.74e-4
Methanol	3.01e-3 kg	0.00225
Natural gas (heating)	1.09e-2 kg	0.0299
Electricity	1.25e-2 kWh	0.0149; 0.0085
Transportation of chemicals and methanol	0.85 kg*km (Est.)	1.64e-4
Outputs – Transesterification only		
Biodiesel	1.00 kg	
Glycerol (>98% purity)	0.106 kg	
Lost biofuel (0.164 kg lost biodiesel, 0.0127 kg glycerol and 0.0802 kg methanol)	0.256 kg	
Waste water for treatment	0.782 kg	0.00258
Outputs – Esterification and transesterification		
Biodiesel	1.02 kg	
Glycerol (>98% purity)	0.106 kg	
Lost biofuel (as above)	0.256 kg (Calc.)	
Waste water for treatment	0.762 kg	0.00251

2.2.2. Increased production of alternative feed products (2)

To analyze how the composition of the poultry feed is changed when not including PF a simulation based on least cost feed optimization (Bestmix Feed Formulation Software, version 3.16) was made. Input for this simulation was prices of feed ingredients, and a restriction of maximum 20 and 25 g kg^{-1} of linoleic acid (C18:2) per kg feed. The content of linoleic acid is limited as even though a high content may improve digestibility and consequently the energetic value, which is an advantage, especially for young animals with limited digestive capacity, the drawback of high unsaturated fatty acid content is the risk of soft fat in broilers at slaughter.

The results showed that the total fat content in the feed remained very constant when PF was removed from the feed, through the increased input of other fat sources. Usable alternatives were assumed to be palm oil and soybean oil. Firman (2006) states that apart from these two oils, sunflower oil is also commonly used in poultry feed. However, due to its higher price, this oil was not considered. The feed simulation showed that for each kg of PF removed from the feed, an input of 0.67 kg of palm oil and 0.34 kg of soybean oil was required, regardless of which limit of linoleic acid in the feed was used. These amounts may be affected by changes in the price of the fats or the energetic value used in the feed, however, the conclusion that PF is replaced by other fats without significant changes in the rest of the diet composition was stable in the simulations. As a small comment, it is interesting to note that the substitution of the PF calls for the production of almost the exact same amount of other types of oil, which are also frequently used for biodiesel. If all other things were equal this would imply that results equal to those of biodiesel based on palm or soybean oil could be expected from this study (Table 3).

The emissions related to the production and transport of palm and soybean oil are outlined in Table 3:

2.2.3. Increased or decreased production and use of fuel oil and diesel (3)

As outlined in Table 1 above, biodiesel will substitute diesel, and lost biofuel will substitute fuel oil. The substitution of fuel amounts are in both cases made on a one-to-one energy (LHV) basis. In relation to the substitution of diesel with PF biodiesel, this assumption is supported in literature (Lapuerta et al., 2008). No literature addresses the efficiency of substituting fuel oil with the lost biofuel, however, the potential inaccuracy introduced by this

Table 3
GHG emissions related to the production of palm and soybean oil needed to substitute 1.16 kg PF.

Oil	Production (kg CO2 eq./kg oil)	LUC emissions (kg CO2 eq./kg oil)	C absorption during growth ($kg\ CO_2$ eq./kg oil	Transportation ($kg\ CO_2$ eq./kg oil)	Needed oil to displace 1.16 kg PF (kg oil)	Total emission to displace 1.16 kg PF ($kg\ CO_2$ eq./kg oil)
Palm:	0.595 (Souza et al., 2010)	2.06 (Croezen et al., 2010)	2.81 (calc. from Metha and Anad, 2009)	0.152[a]	0.777	0.167
Soy:	1.16 (Ecoinvent, 2007)	2.03 (Croezen et al., 2010)	2.84 (calc. from Metha and Anad, 2009)	0.0745[a]	0.394	

[a] The emissions from transportation are based on the assumption that the palm oil comes from SE Asia. In SE Asia, the average distance from the oil mill to the harbor is assumed to be 500 km on rail. Sailing distances from SE Asia across the Atlantic Ocean to the US east coast, is estimated to be 19,000 km. The east coast rather than the west coast is chosen because the biofuel plant used in this case study is located close to the east coast (see Section 2.2.1) and because the PF displaced is assumed to be produced relatively close to the biofuel plant, implying that palm oil transported to the west coast would not be able to substitute PF close to the east coast without being transported across the US, which is considered less likely. The distance from the US east coast harbor to the biodiesel plant is 500 km, which is done by rail. Soybean oil is assumed to be produced in the in the largest soybean producing states in the US, calling for around 1500 km of transportation by rail to the feed producer.

assumption will be very limited. Below, Table 4 summarizes the substituted amounts and the resulting GHG emissions. The GHG emissions are calculated by summing the emissions from production and use of the fuels. The GHG emission from the use of the fuels will vary as the chemical composition of e.g. diesel and biodiesel differs. This difference in emissions from the use is calculated through first calculating the mass of the substitutes. Then the carbon content of each of these masses is calculated based on average molecular structure and converted to CO_2, and the numbers for the substituting and the substituted fuel are subtracted. The numbers below show the total GHG emission, including production and use emissions. Emissions from the production are based on standard process data (Ecoinvent, 2007) (Table 4).

Transportation distances from the poultry rendering plant or biodiesel plant to the user is assumed equal to the distances from the refinery to the user. Therefore, no changes in emissions from transportation are assumed.

2.2.4. Glycerol used in the production of PG (4)

As mentioned above, glycerol can be used in the production of PG, and is thereby assumed to substitute petrochemically produced PG. The production of PG from glycerol includes a catalytic dehydration to acetol and a catalytic hydrogenation and distillation to PG (Pagliaro and Rossi, 2010). No standard data for this process could be found, so an estimate of the related GHG emissions based on the included processes was performed. The glycerol is heated to 200 °C (from an assumed ambient temperature of 20 °C) under close to atmospheric pressure (Pagliaro and Rossi, 2010). The heating is assumed to be performed by natural gas with 90% efficiency. With a specific heat of 2.4 kJ/(kg K) and a mass of 0.106 kg glycerol, this gives an emission of 0.0035 kg CO_2 eq (Ecoinvent, 2007). The resulting acetol is hydrogenated using 1 mol of H_2 per mol of acetol, resulting in 0.0047 kg CO_2 eq (Ecoinvent, 2007). Finally, the PG is distilled, using natural gas, as before. Assuming no energy for cooling and a heat of evaporation of 67 kJ mol^{-1}, this results in an emission of 0.0071 kg CO_2 eq (Ecoinvent, 2007). The petrochemical production of 0.106 kg PG results in 0.441 kg CO_2 eq (Ecoinvent, 2007). Substituting petrochemical PG with PG based on glycerol thereby results in a saved emission of 0.426 kg CO_2 eq. It should be noted that in reality the saved emissions is probably a little lower, as the production is assumed to run at a 100% efficiency in terms of hydrogen input and without the use of auxiliaries, such as catalysts and electricity. The transport of the petrochemical PG and the PG based on glycerol are assumed to be equal and thereby not lead to any changes in GHG emissions.

2.2.5. Glycerol substituting feed (5)

A second possibility mentioned in literature is the use of glycerol as energy feed. The marginal energy feed is assumed to be wheat (Bauen et al., 2010). 1 kg of glycerol has been reported to have the same feed energy as 0.938 kg of wheat (Jonasson and Sandén, 2004).

GHG emissions related to the production of wheat is assumed to be 0.685 kg CO_2 eq./kg (Ecoinvent, 2007). The average land use change emissions related to the production of wheat is 0.443 kg CO_2 eq./kg (Croezen et al., 2010) (calculated from land use change emissions from wheat ethanol (Bernesson et al., 2006), using a 20 year amortization period). The uptake of CO_2 during growth is around 1.58 kg CO_2/kg wheat (carbon content is around 43% (Merah et al., 1999)). In total, the production of 1 kg of wheat absorbs 0.452 kg CO_2. Assuming that the GHG emissions from the livestock are equal whether they are fed with wheat or glycerol, this implies that substituting 0.106 kg of glycerol with wheat results in an emission of 0.0449 kg CO_2 eq. The transportation of the glycerol and the wheat is assumed to be equal.

3. Results

Based on the above findings 8 different scenarios have been developed by combining in all possible ways each of the two outcomes for each of the 3 scenario variables; the two different uses of the glycerol resulting from the production of biodiesel, the two different biodiesel production processes, and the two different marginal electricities.

The results for these scenarios are shown below.

The 'total' for each scenario fluctuates around an average of −6%, indicating that the total emissions in the 'new situation' where PF is used for biodiesel are on average slightly lower than in the baseline situation (where the PF is used for original purposes and

Table 4
GHG emissions from substitutions and use of fuels. Negative total GHG emissions indicate that using biodiesel or lost biofuel instead of diesel or fuel oil lowers emissions.

Substitution	Fuel	Energy content (MJ/kg)	Masses substituted (kg)	Carbon content (w. C/w. total)	Production ($kg\ CO_2$ eq.)	Total GHG emission ($kg\ CO_2$ eq.)
Diesel with PF biodiesel	Diesel:	42.5	0.886	0.861	0.531	−0.50
	PF biodiesel:	37.7	1	0.771	Incl. above	
Fuel oil with lost biofuel	Fuel oil:	44.6	0.181	0.861	0.088	−0.070
	Lost biofuel:	31.5	0.256	0.628	Incl. above	

Table 5
Well-to-wheel GHG emissions for the use of PF biodiesel. The table shows the 8 included scenarios, developed by varying the 3 scenario variables in all possible ways. A number in a cell indicates that a certain outcome of a scenario variable is considered for the given scenario number. For example, in scenario 1, it is assumed that the produced glycerol will substitute PG; that the electricity used in the biodiesel process is based on coal; and that the biodiesel production does not include an esterification process. Furthermore, as all scenarios, scenario 1 includes emissions related to the substitution of PF, the substitution of diesel with PG biodiesel, and the substitution of fuel oil with 'biofuel'. A total emission of zero would indicate that there are no difference in the total emissions from the baseline situation and the new situation where PF is used for biodiesel. Negative numbers indicate avoided emissions.

Scenario variable	Scenario number and GHG emission per kg of biodiesel (kg CO_2 eq., negative number indicate saving)							
	1	2	3	4	5	6	7	8
Feed substitute PF	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16
Glycerol used for PG and substitute pet. PG, no purification of glycerol	−0.43		−0.43		−0.43		−0.43	
Glycerol substitute feed		0.04		0.04		0.04		0.04
Biodiesel production includes esterification, coal			0.46	0.49				
Biodiesel production excludes esterification, coal	0.39	0.42						
Biodiesel production includes esterification, natural gas							0.37	0.40
Biodiesel production excludes esterification, natural gas					0.31	0.34		
Biodiesel substitute diesel	−0.50	−0.50	−0.50	−0.50	−0.50	−0.50	−0.50	−0.50
Biofuel substitute fuel oil	−0.07	−0.07	−0.07	−0.07	−0.07	−0.07	−0.07	−0.07
Total	*−0.45*	*0.05*	*−0.38*	*0.12*	*−0.53*	*−0.03*	*−0.47*	*0.03*
Compared to driving on diesel[a] (%) (negative number indicate saving)	*−13*	*2*	*−11*	*4*	*−16*	*−1*	*−14*	*1*

[a] See footnote 3.

petrochemical diesel is used). This implies that according to this assessment, using PF in the production of biodiesel does in most assessed cases lead to a small reduction in GHG emissions. Using PG biodiesel will in the most positive scenario above reduce emissions by 15% in comparison to driving on petrochemical diesel[3], in the most negative scenario lead to an increase in GHG emissions of 4%.

The variation between the scenarios is mainly explained by what the glycerol substitutes. From the most positive to the most negative case, this results in difference of 15% in comparison to driving on diesel. Which of these substitutions is the most likely, however, is difficult to assess as the various solutions to the utilization of the glycerol produced in the biodiesel production are still being analyzed (Pagliaro and Rossi, 2010).

The results also point to that the increased efficiency of the process by including an esterification process in this case does not fully compensate the increase in GHG emissions from the increased use of chemicals and energy in the biodiesel production process. However, it should be mentioned that sulfuric acid esterification is normally done for oils with higher content of FFA than the PF used in this study, and in these cases, the situation may be different.

Whether the electricity input to the biodiesel production is based on coal or natural gas shows to have a relatively small but noticeable effect. The emissions from the 'natural gas' scenarios have around 2% lower GHG emissions than scenarios based on coal.

Besides the variation in the scenario results, there are significant uncertainties related to several of the emissions included in this assessment. A major uncertainty relates to the land use change emissions from the production of palm and soybean oil and, to a lesser extent, wheat. This study has used average values from literature with a 20 year amortization period. Varying these land use change emissions, both through using maximum and minimum reported emissions (Croezen et al., 2010), and through the use of a 30 year amortization period, which is often used in US studies, the final results from scenario 2 would vary from 25% to −37% in comparison to driving on diesel.

A second uncertainty relates, as mentioned above, to what the glycerol from biodiesel will actually substitute. To analyze the importance of this uncertainty in more depth, we have included the potential substitution of petrochemical glycerol and power plant fuel with glycerol. If substituting petrochemical glycerol on a one-to-one weight basis, and using standard process data (Ecoinvent, 2007) the final results in scenario 1 would be −16% (instead of −13%) in comparison to driving on diesel. If on the other hand glycerol substitutes fuel oil in power plants on a one-to-one LHV basis using standard process data (Ecoinvent, 2007) the final results in scenario 2 would be 1% lower (i.e. 1% in comparison to driving on diesel). What glycerol substitutes can thereby make a significant difference, but this shows that the inclusion of these additional substitution possibilities does only slightly add to the variation already considered in the scenarios above.

Changes in the efficiency of the process may also influence the results significantly. Comparing to a 100% efficient process, here understood as a process where all oil is either converted to biodiesel and glycerol in proportionate amounts and the input of methanol is based on stoichiometric calculations, the results would be lowered by around 5% in comparison to driving on diesel due to the lowered input of oil, and by 3% due to the lowered consumption of methanol. However, at the same time, no lost biofuel would be produced, as it is only produced when the biodiesel production is not running with 100% efficiency. And as the lost biofuel substitutes fuel oil, this lowered output of lost biofuel would increase the total emission of 2%, giving a reduction potential of around 6% in total. This potential may be lowered by 1% extra if also considering the potential use of catalyst residue as a fertilizer, as considered in Jensen et al. (2007). If also using the somewhat lower power consumption considered by Jensen et al. (2007) an additional ½% may be gained. In total, this implies that a fully optimized process could decrease the GHG emissions by around 7.5% in comparison to driving on diesel.

Another and much smaller uncertainty relates to the assumptions about transportation of the palm and soybean oils in Section 2.2.2. Here it was among other assumed that the palm oil in SE Asia is transported 500 km by rail to the harbor. As this may vary quite significantly, a doubling and halving of the distance was considered. The other distances included are considered to be more robust, given the explanations in Section 2.2.2. Incorporating this lower demand for transportation in scenario 1 will lower the emissions by 0.2% in comparison to driving on diesel, whereas incorporating the higher transport demand will increase the emission by 0.4%.

This indicates that in an absolute best case, using minimum land use change emissions, a fully optimized process, best substitution

[3] The well-to-wheel emission from the combustion of 1 MJ of diesel in a car engine is 0.0896 kg CO_2 eq. (Ecoinvent, 2007). One kg of PF biodiesel contains 37.7 MJ. To obtain 37.7 MJ of energy from diesel results in 3.38 kg CO_2 eq.

of glycerol, and minimizing transportation the result in scenario 5 would be −64% in comparison to driving on diesel. Similarly, in the 'worst case', where the efficiencies of the process are as presented in this study, where the transportation demand is high, and where land use change emissions are at a reported maximum, the emissions in scenario 4 would be 26% higher than when driving on diesel. However, as a comment to this, it should be noted that the emissions on which the scenarios in Table 5 are based are considered average, and that the lower and upper value should be considered as 'extremes'.

Besides these and several other uncertainties relating to the processes included in the scenarios, there are other and probably much larger uncertainties related to whether the futures considered in these scenarios will actually materialize. We have here assessed scenarios which are based on a variety of actual or earlier events, but despite our attempts to foresee different futures by combining these variations in different ways, the future often shows difficult to predict. Even though we have attempted to find the most realistic market responses, others than the ones considered here is therefore a possibility. How this can change the results is impossible to say.

4. Discussion and conclusions

Many other LCAs on BPO have been performed, as mentioned in Section 1, and where it is possible to compare, these studies often get to very different results. Several explanations may be given for these differences, such as different type of BPO used, geographical setting, process efficiencies, etc. However, a main difference is that in many studies the use of the BPO for biodiesel is considered not to lead to any substitutions. At the same time, when burned in the engine, the GHG emissions are assumed biogenic, and therefore zero. Had it been assumed in this study that the use of the BPO did not lead to any substitutions, the result in scenario 1 would be around −101% in comparison to driving on diesel. These assumptions about substitutions are therefore very important for the results. Given that the use of BPO actually leads to an increased production of a substitute, as assumed in this study, and if the purpose of the study is to answer the "what happens if…?" type of question as addressed in this study, then these concerns need to be included in the assessment. Some may argue that this is only relevant if following a 'consequential LCA' and when applying an 'attributional LCA' approach these concerns do not need to be included. The terms 'attributional' and 'consequential' have deliberately not been used in this article. Rather than claiming to belonging to a certain 'LCA school', this article has simply attempted to answer the question: Is it beneficial in terms of GHG emissions to use PF biodiesel? If this is what the assessment attempts to answer then these very central emissions cannot be ignored simply by referring to a methodological choice.

Considering that a central focus in the biodiesel debate is its potential to reduce GHG emissions, answering "what happens if…?" seems central. As argued above, in relation to BPO biodiesel this entails a consideration of the alternative use of BPO. Besides this study, this has only been done in two studies. Jensen et al. (2007) have assessed the GHG emissions from biodiesel made from rendered fats in general (reaching very similar results as found here when taking into account the differences in the cases), and Nelson and Schrock (2006) assesses biodiesel made from beef tallow, but does not include GHG emissions. As several other types of BPO exist, this therefore seems as a relevant area for future research.

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Appendix F: Sustainable biodiesel based on enzymes [Bæredygtig biodiesel med enzyme]

Authors: Mathias Nordblad, Yuan Xu; Ivan Tengbjerg Herrmann, Michael Zwicky Hauschild; Thomas Jensen, Jesper Brask, and John Woodley

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Bæredygtig biodiesel med enzymer

Enzymteknologi åbner nye muligheder for en mere bæredygtig biodiesel, sammenlignet med teknologien vi anvender i dag

Af Mathias Nordblad[1], Yuan Xu[1], Ivan T. Herrmann[2], Michael Hauschild[2], Thomas Jensen[3], Jesper Brask[4] og John M. Woodley[1]
[1]DTU Kemiteknik, [2]DTU Management, [3]Emmelev A/S, [4]Novozymes A/S

Biobrændstof, herunder biodiesel, er en vigtig brik i puslespillet om at nedbringe transportsektorens CO_2-udslip. Andre brikker er alternative transportformer, mere energirigtige biler og på længere sigt el- og hydrogenbiler. På trods af at biodiesel baseres på vedvarende råstoffer, er bæredygtigheden til debat. I et nyt projekt ("Sustainable Biodiesel" støttet af Højteknologifonden) mellem DTU, Aarhus Universitet, Novozymes A/S og Emmelev A/S er målet at udvikle en mere bæredygtig biodiesel (faktaboks 1). Nøglen er at bruge enzymteknologi i produktionsprocessen.

Biodiesel produceres i dag fra triglycerider og frie fedtsyrer ved forestring/alkoholyse med methanol (faktaboks 2, side 12). Det er tidligere blevet foreslået at benytte planteolier direkte i dieselmotorer. Konverteringen af glyceriderne til mindre fedtsyreestre (methylestre, FAME; ethylestre, FAEE) nedsætter dog dramatisk viskositeten, hvilket giver en renere forbrænding (specielt i koldere egne). Dette blev udviklet op gennem 1990'erne, og biodiesel er i dag defineret som FAME i europæiske og amerikanske normer.

Figur 1. Positive miljøpåvirkninger med enzymatisk FAEE-produktion.

Faktaboks 1. "Sustainable Biodiesel"-projektet

"Sustainable Biodiesel" er et samarbejde mellem DTU Kemiteknik og DTU Management, Aarhus Universitet, Emmelev A/S samt Novozymes A/S. Projektet, der begyndte i september 2008 og løber i 3½ år, har et total budget på 33 mio. kr., hvoraf Højteknologifonden bidrager med 17 mio. kr. Formålet med projektet er at udvikle teknologien til produktion af næste generation bæredygtig biodiesel, komplet med kvantitativ dokumentation af miljøbelastningerne. Arbejdsfordelingen mellem partnerne er som skitseret nedenstående:

- DTU Kemiteknik. Gruppen ledet af John Woodley vil fokusere på procesdesign, herunder at bestemme den optimale reaktortype.
- DTU Management. Gruppen ledet af Michael Hauschild er ansvarlig for livscyklusvurderinger (LCA) af den/de udviklede processer.
- Aarhus Universitet, Molekylærbiologisk institut. Xubing Xu's gruppe vil bidrage med fundamentale studier af enzymkinetik og analysemetoder.
- Emmelev A/S. Emmelev er en dansk biodieselproducent, hvis bidrag til projektet i form af markedsindsigt og vareprøver, vil komme til at spille en stor rolle.
- Novozymes A/S. Udvikler de immobiliserede enzymer der skal erstatte de kemiske katalysatorer i biodieselprocessen.

Al den biodiesel, der fremstilles i dag (ca. 10 mio. tons), er produceret med kemisk katalyse. Det er en simpel og velfungerende reaktion for rene planteolier. Udfordringen for de kemiske katalysatorer kommer, når lavkvalitetsolier benyttes som råmateriale, idet der så skal benyttes både en sur og en basisk katalysator. Desuden virker de kemiske katalysatorer bedst med methanol (FAME), mens ethanol (FAEE) giver en række problemer med vandindhold og langsomme reaktioner. Enzymer (lipaser) kan være løsningen på disse problemer.

Man har længe kendt til teknologien omkring anvendelsen af enzymer som biokatalysatorer til fremstillingen af biodiesel. En stor fordel med enzymatisk produktion af biodiesel er, at man i en forholdsvis simpel proces kan omdanne olier, inkl. lavkvalitetsolier med højt indhold af frie fedtsyrer, til biodiesel. Andre fordele, som vist i figur 1, inkluderer et lavere energi- og vandforbrug, substitution af stærke syrer og baser med en biologisk katalysator, at biproduktet glycerol kommer rent ud, samt de forbedrede muligheder for at anvende bioethanol i stedet for methanol.

Men den helt store udfordring mht. enzymatisk biodiesel er, at kunne opskalere en sådan proces og samtidig gøre den økonomisk rentabel.

Olier

Udgiften til rene, vegetabilske olier er typisk op mod 85% af de totale biodiesel produktionsomkostninger. Der er således en stor gevinst at hente, hvis lavkvalitets (lavpris)-olier kan udnyttes [1]. Når der er et marked for biodiesel fra rene olier, skyldes det statslige tilskudsordninger og regler for obligatorisk iblanding. Biodiesel kan i dag ikke konkurrere med fossil diesel på prisen. Også fra et miljømæssigt synspunkt vil det utvivlsomt være en fordel at gå fra madolier til spildolier. Det kan blot ikke erstatte hele biodieselproduktionen, da mængderne (af eksempelvis brugt fritureolie) er for små.

De vigtigste planteolier til biodiesel er soja-, raps-, palme- og jatrophaolier. De fleste af de tilgængelige vegetabilske olier er almindelige madolier. Jatrophaolie anvendes ikke til madproduktion, men dyrkes specifikt med henblik på biodieselproduktion i store områder i lande såsom Kina og Indien. Selvom man i fremtiden med gensplejsning har udsigt til at udvikle afgrøder med et højt indhold af olie [2], vil der stadig være debat om brug af fødevarer og landbrugsjord til brændstof.

Et andet interessant og lovende råmateriale er olie udvundet fra mikroalger, der potentielt kan produceres i meget stor skala, idet mikroalger gror ekstremt hurtigt og udnytter sollys mere effektivt end planter [3]. Endvidere har mikroalger den klare fordel, at de ikke konkurrerer med andre afgrøder om landbrugsjorden.

Alkoholer

Methanol anvendes i dag i stor skala i biodieselproduktionen. Et af målene med "Sustainable Biodiesel"-projektet er at erstatte denne methanol med (bio)ethanol, hvilket vil give en række fordele:

- Med bioethanol fås et 100% biobrændstof (med FAME er det kun oliedelen, der er "bio").
- Ethanol er mindre giftigt end methanol.
- Ethanol er mere kompatibelt med en enzymatisk proces end methanol.
- Med øget bioethanolproduktion og stigende oliepriser kan det forventes, at prisforskellen mellem ethanol og methanol vil falde.
- FAME og FAEE har stort set identiske egenskaber, men det teoretiske FAEE-produktionsudbytte fra 1 kg olie er større end det tilsvarende FAME-udbytte (pga. den større molvægt af ethanol).

Enzymer

For at gøre en enzymatisk biodieselproces økonomisk rentabel er det nødvendigt, at enzymerne genanvendes. Den letteste måde at gøre det på er ved at benytte immobiliserede enzymer, hvor enzymerne sidder fast på og i små porøse partikler (typisk 0,1–1 mm i diameter). Partiklerne kan være uorganiske materialer (f.eks. silika) eller plastpolymere (f.eks. polystyren). Immobiliserede enzymer kan således genbruges efter en simpel filtrering af reaktionsblandingen, eller de kan pakkes i kolonner til brug i en kontinuerlig proces. Desuden har immobilisering generelt en positiv effekt på enzymernes stabilitet (over for solventer og høje temperaturer), ligesom immobilisering gør selve håndteringen lettere. Endelig, i modsætning til enzymer i vandig opløsning, kan immobiliserede enzymer tilsættes uden der samtidig introduceres vand i systemet. Immobiliserede lipaser anvendes allerede i dag i stor skala i fedt- og olieindustrien til interesterificering af triglycerider i fremstillingen af margarine (for at tilpasse smeltepunktet) [4].

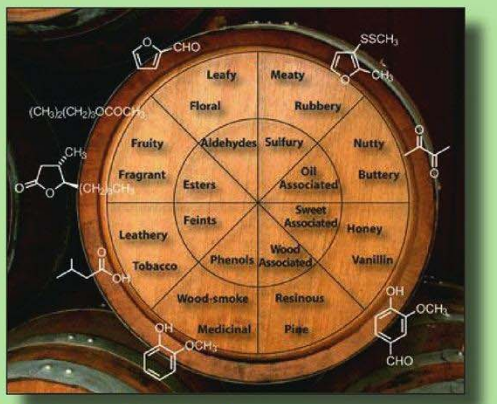
For at gøre en enzymatisk biodieselproces rentabel er det afgørende at sikre en god levetid af de immobiliserede enzymer.

Figur 2. Emmelev A/S er en dansk biodieselproducent. Produktionen er i dag baseret på rapsolie og traditionel kemisk katalyse.

Flere faktorer påvirker levetiden, herunder urenheder i olien (oxidationsprodukter m.m.), alkoholen, temperaturen, glycerol og vandkoncentration [5]. Generelt er immobiliserede enzymer dyrere end flydende enzymer. Den immobiliserede lipase Novozym 435, som benyttes i mange publikationer med enzymatisk biodiesel, har en meget høj kg-pris, hvilket kræver en meget høj produktivitet (kg biodiesel pr. kg enzym), før processen bliver rentabel. Novozymes' bidrag til "Sustainable Biodiesel"-projektet bliver således at udvikle kost-effektive immobiliserede enzymsystemer.

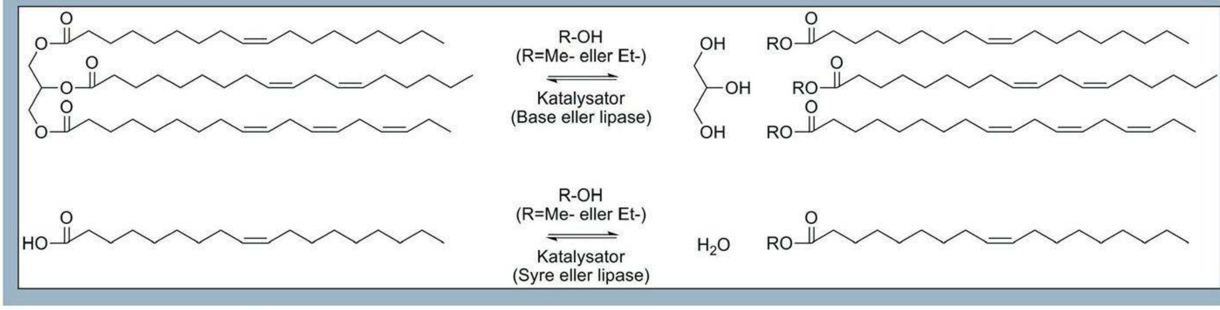
Reaktorteknologi

Immobiliserede enzymer introducerer en fast fase i systemet. Der kan endvidere være flere flydende faser, idet alkohol (methanol eller ethanol), vand og glycerol (hhv. reaktanter og produkter)



Faktaboks 2. Biodieselreaktionen

Biodiesel produceres ud fra planteolie eller (i enkelte tilfælde) animalsk fedt. Råmaterialet består derfor af triglycerider med et varierende indhold af di- og monoglycerider, samt frie fedtsyrer. I biodieselreaktionen reagerer disse komponenter med methanol, hvorved der dannes fedtsyremethylestre (FAME), glycerol og vand. Alkoholysen af glyceriderne katalyseres traditionelt af en base så som NaOH eller $NaOCH_3$, mens forestringen af de frie fedtsyrer traditionelt katalyseres surt af H_2SO_4. Alternativt kan alle reaktionerne katalyseres af enzymer (lipaser), ligesom det i projektet foreslås at erstatte methanol med (bio)ethanol. Det resulterende biobrændstof bliver således fedtsyreethylestre (FAEE). Figuren illustrerer tre hyppigt forekommende fedtsyrer i planteolier: oliesyre (C18:1), linolsyre (C18:2) og linolensyre (C18:3).



alle har ringe opløselighed i olie. For at sikre høj reaktionshastighed er der brug for en god kontakt imellem det immobiliserede enzym og reaktanterne. Under betingelser hvor der kun er en homogen flydende fase, er en kolonne pakket med immobiliseret enzym (en packed-bed reaktor) et åbenlyst valg. Denne reaktortype er dog problematisk, hvor der er flere flydende faser. I dette tilfælde er en omrørt tankreaktor nok mest velegnet. Efter reaktionen er det nødvendigt at oprense reaktionsblandingen, typisk ved at en glycerolfase separeres og overskydende alkohol dampes af og genanvendes. Separationen og videre processering af biproduktet glycerol er også interessant, da det er et værdifuldt kemikalie med en række anvendelser i den kemiske og farmaceutiske industri. Opsætningen af den bedst tænkelige reaktorteknologi og operative strategi er hovedformålet for DTU Kemiteknik.

Miljøpåvirkning

Med enzymatisk fremstilling af biodiesel er der gode chancer for, at man kan reducere de negative påvirkninger af vores miljø sammenlignet med den traditionelle kemisk katalyserede FAME-proces. Ud over bidrag til den globale opvarmning drejer det sig også om andre påvirkningskategorier som bl.a. forsuring og økotoksitet.

Når man vil vurdere miljøpåvirkningen fra et produkt, en proces eller en teknologi, er det vigtigt at anlægge et "vugge til grav"-perspektiv gennem en livscyklusvurdering (LCA). Hvis man blot ser på miljøpåvirkningerne i en brugsfase, overser man de miljøpåvirkninger, der finder sted i produktionsfasen eller i bortskaffelsesfasen, og man foretager let en suboptimering, hvor miljøbelastningen bare forskydes væk fra den del af livscyklusen, man ser på.

I et livscyklusperspektiv viser indledende studier af biodieselproduktion med enzymer som katalysator for transesterificeringsprocessen af eksempelvis rapsolie, at miljøpåvirkningerne kan reduceres ift. konventionel biodieselproduktion [6]. I sammenligningen med almindelig petrokemisk baseret diesel har biodiesel fordele inden for de fleste af de emissionsrelaterede miljøpåvirkninger, især den globale opvarmning. Til gengæld har konventionel diesel en fordel i påvirkningskategorien "arealanvendelse", hvor biodiesel som nævnt kan forårsage en utilsigtet fortrængning af fødevareafgrøder til fordel for olieafgrøder til produktion af biodiesel [7]. I Danmark har vi særdeles veludviklede LCA-kompetencer. Det udnyttes i udviklingen af en enzymatisk biodieselproduktion, der er så bæredygtig som muligt.

E-mail-adresse:
Jesper Brask: jebk@novozymes.com

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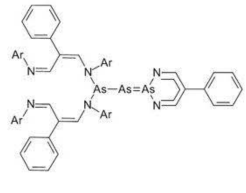
Nyt om...

... Tre arsenatomer - tre oxidationstrin



En arsenforbindelse med tre arsenatomer er for nylig blevet beskrevet, dette er usædvanligt. De tre arsenatomer har forskellige oxidationstrin. Det formelle oxidationstrin for de tre arsenatomer i rækkefølgen As-As=As er fra venstre II, 0 og I, yderligere må røntgenstrukturundersøgelser tydes således, at der er en As=As-binding, som den man oprindelig troede fandtes i salvarsan, det første middel mod syfilis; men hvad der senere viste sig at være forkert. Alt i alt en usædvanlig forbindelse.

Carl Th.

Diminato complexes of arsenic *Chemical Communication* 2009, side 428